Granular Matter
From granular gases to granular fluids/solids

S. Luding

Multi Scale Mechanics, TS, CTW, UTwente,
POBox 217, 7500 AE Enschede, NL --- s.luding@utwente.nl

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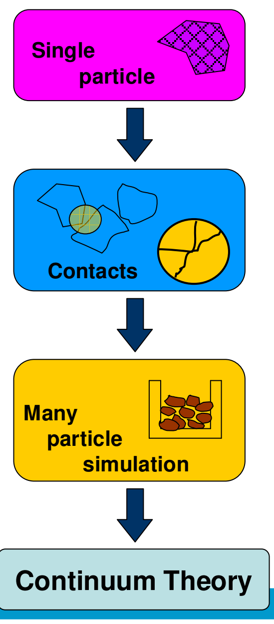
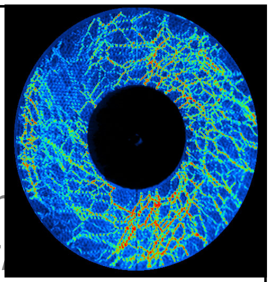


Granular Materials



Numberless applications:

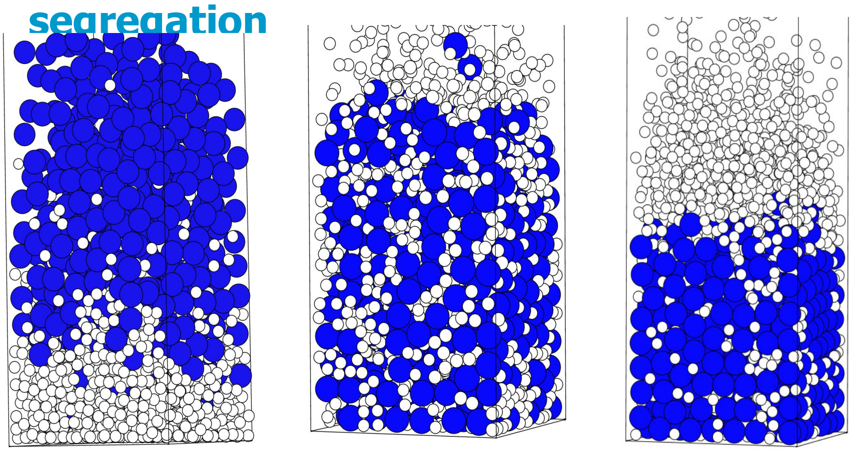
- constructions, industry (silos), agricultur
- everyday life (e.g. coffee powder, sugar,

Challenges for Comp. & Statistical Physics

- many particle system – classical mechanics
- non-linear, non-equilibrium, statistical physics

segregation (mixing), pattern formation (dunes),
force chains (wide distributions)
localization (shearbands, avalanches, clusters)

Segregation – Mixing – Reverse segregation



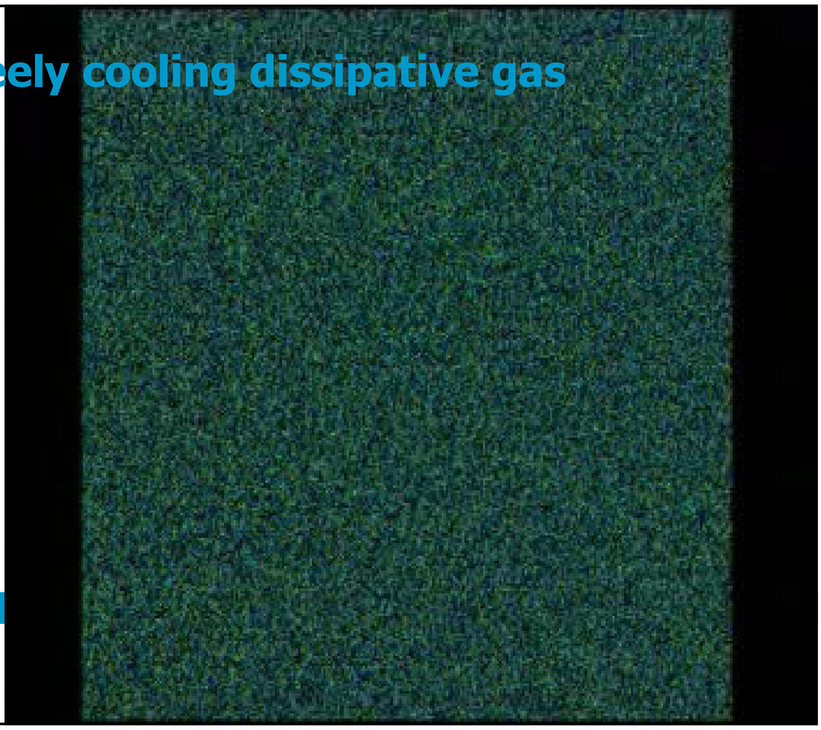
P. V. Quinn, D. Hong, SL, PRL 2001

Clustering
- (weakly) vibrated box with compartments

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

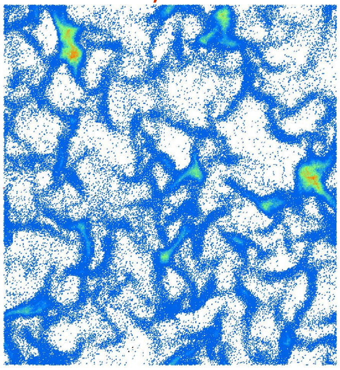
Freely cooling dissipative gas

2D



How to understand clustering ?

Goldhirsch, Zanetti 1993, …



- Higher density
- More dissipation
- Lower Pressure
- etc.

… is that all ?

… equations of state for all densities

How to approach ?

Continuum theory (micropolar, …)

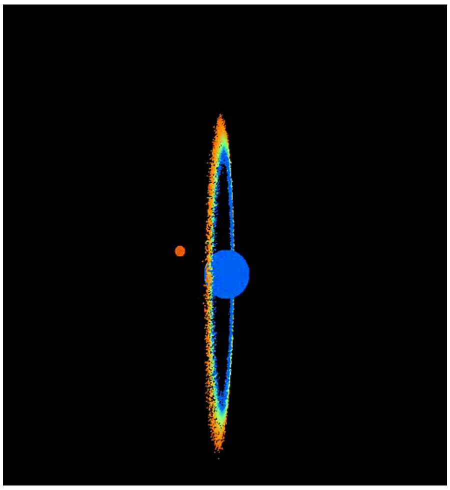
Statistical Physics

+ Kinetic theory + dissipation + friction

Numerical

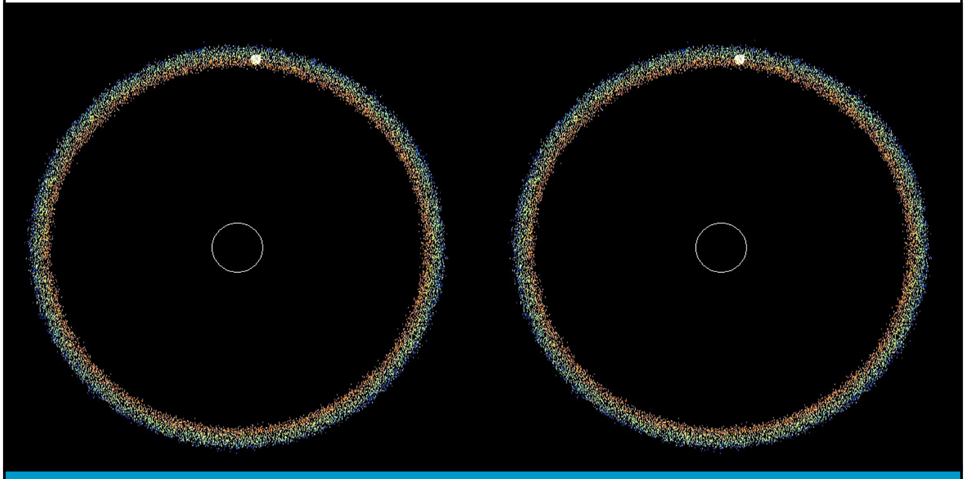
- Monte Carlo (for non-equilibrium ?)
- Molecular dynamics simulations (MD)
- PDEs (FEM, FV or CFD)

Molecular Dynamics example from astrophysics



Examples:

astrophysical clouds, rings



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***

Elastic hard spheres

elastic steady state: $$\frac{\partial}{\partial t}=0 \qquad u_i=I=0$$

mass & energy conservation – OK

momentum balance: $$0=-\frac{\partial}{\partial x_i}P \qquad g_i=0$$

- **Pressure *P***
- **Shear Stress** $\sigma_{ij}^{\text{dev}}=0$
- **Energy Dissipation Rate *I=0***

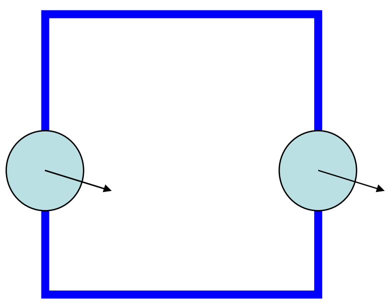
First example … pressure

$$P = \frac{E}{V}\left(1+\left(1+r\right)\nu g_{2a}\left(\nu\right)\right)$$

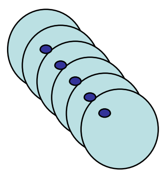
$$g_{2a}\left(\nu\right) = ?$$

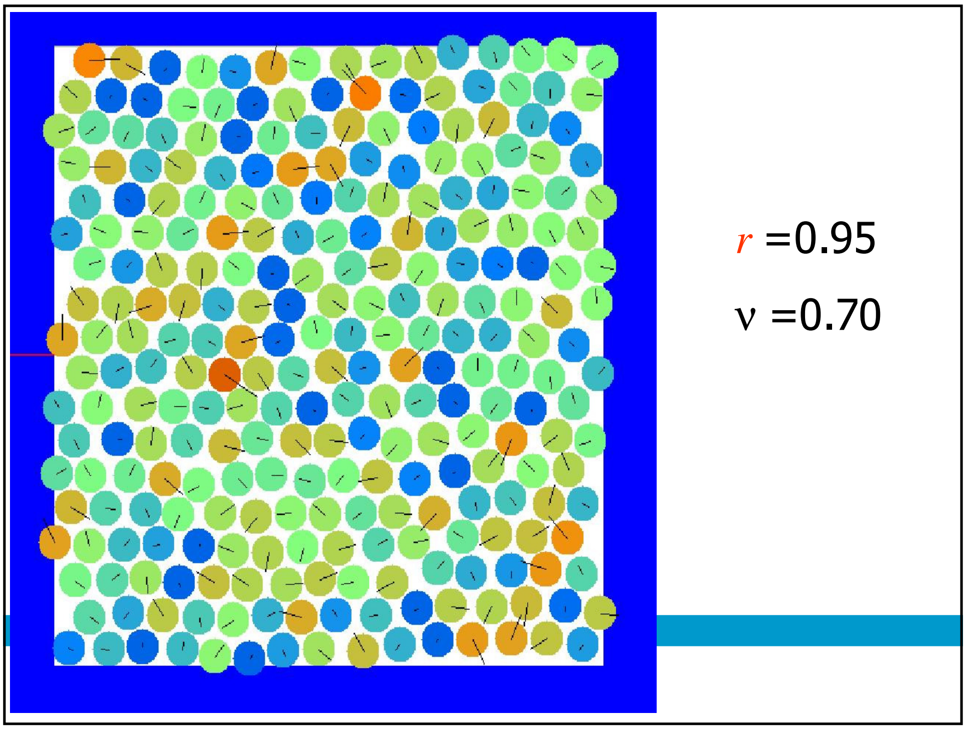
Elastic Hard Sphere Model

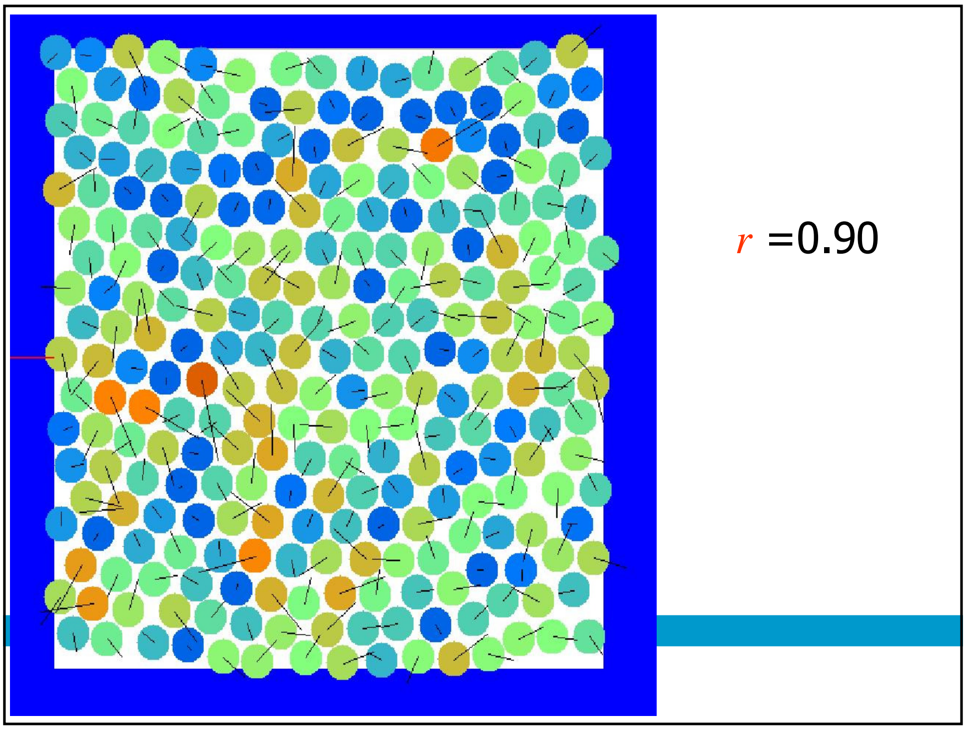
simulate *N* particles
in a peridoc box

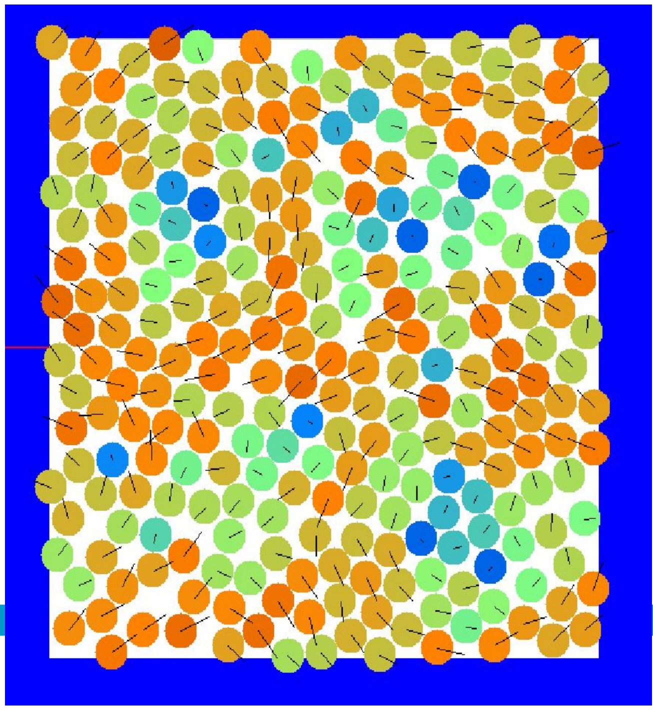


… plot path-lines



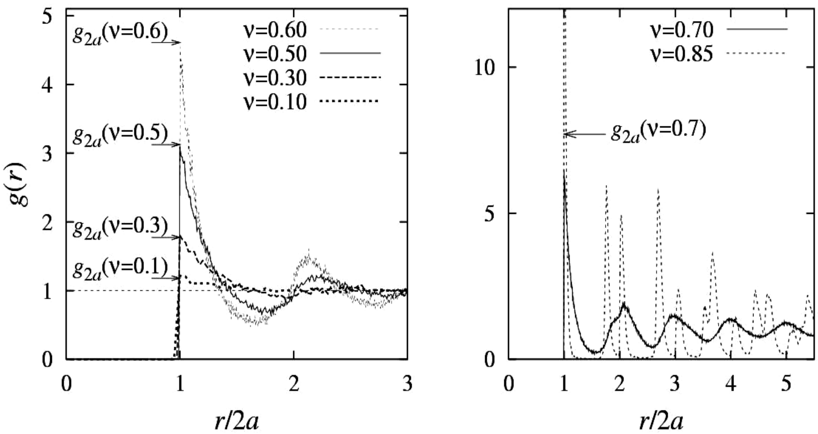

r =0.95
ν =0.70


r =0.90

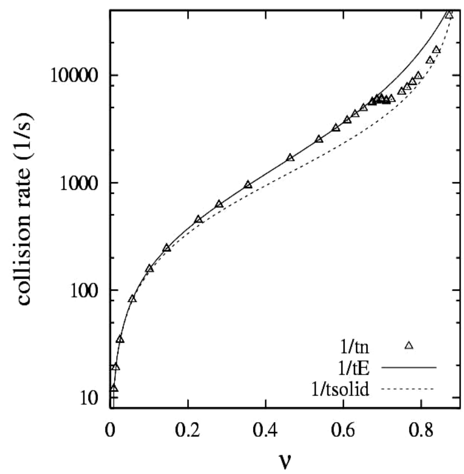


r =0.80

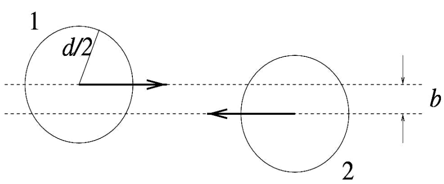
Contact probability – correlation function

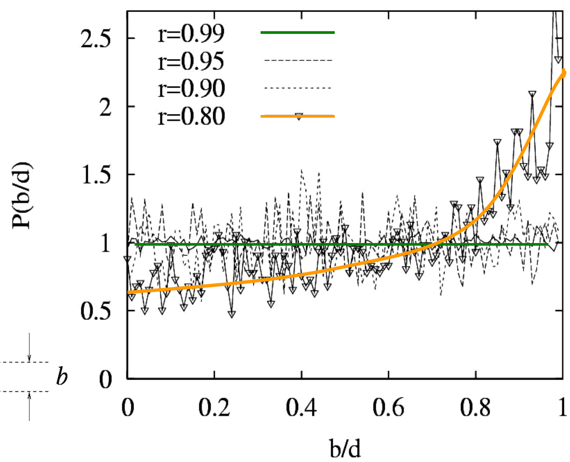


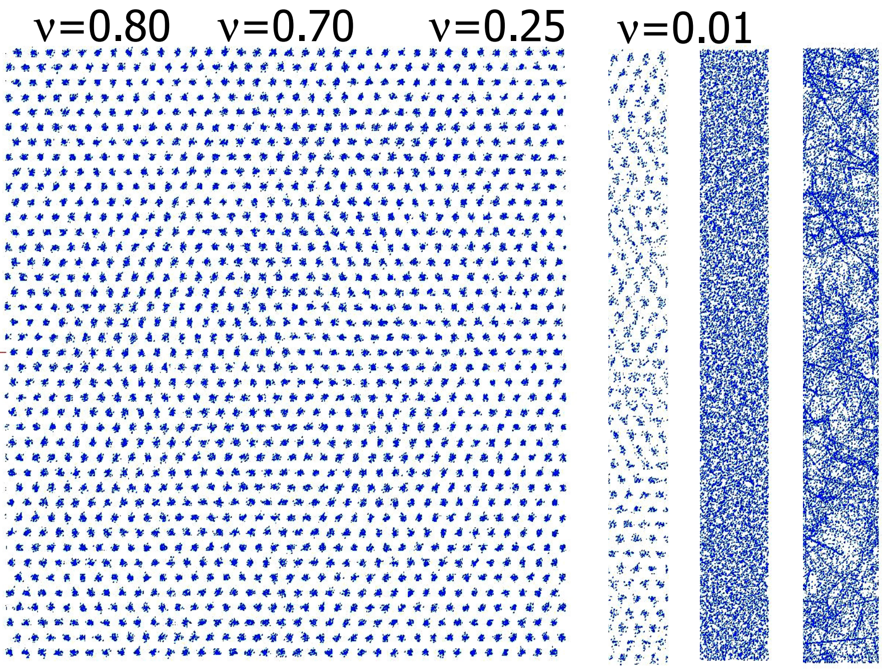
Collision rate – time scale



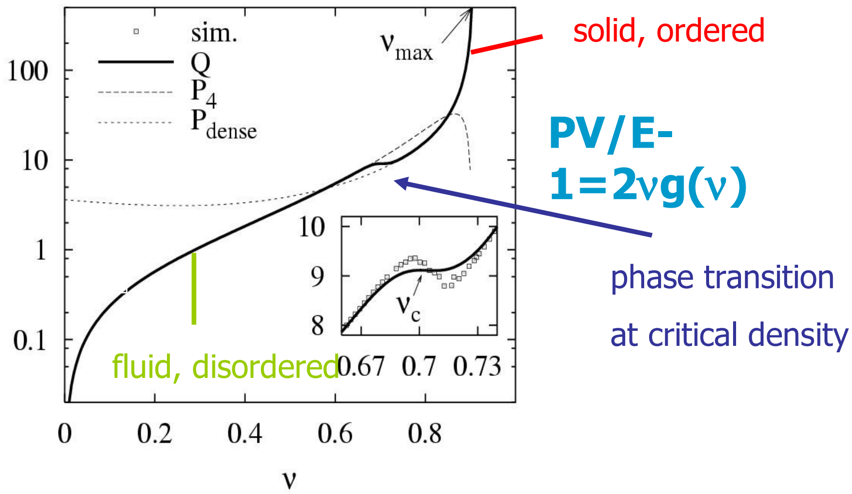
Collision parameter



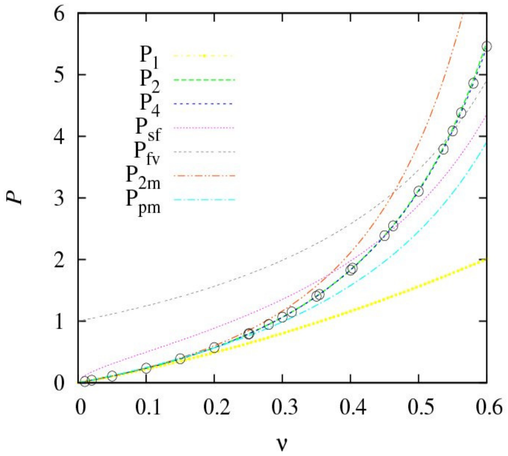




Pressure (Equation of State – 2D)

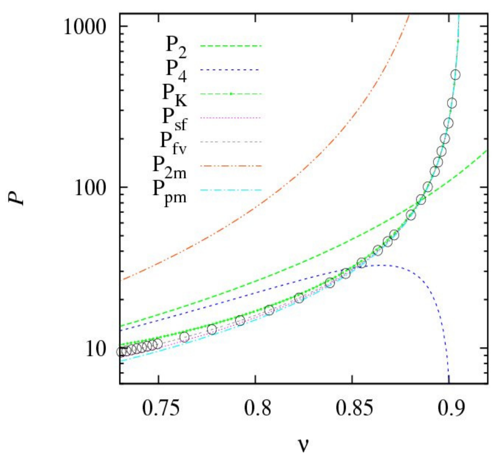


Pressure (Equation of State – 2D)

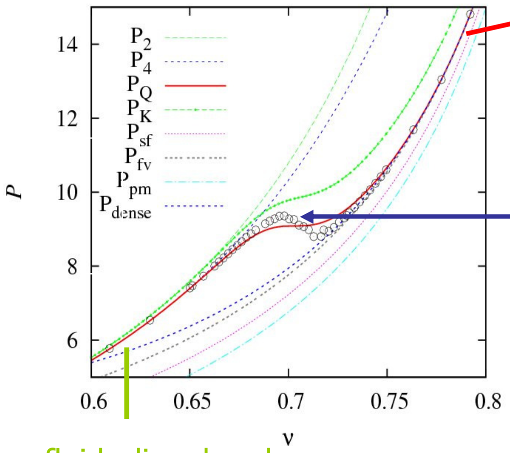


PV/E-1=2νg(ν)

Pressure (Equation of State – 2D)



Pressure (Equation of State – 2D)



solid, ordered

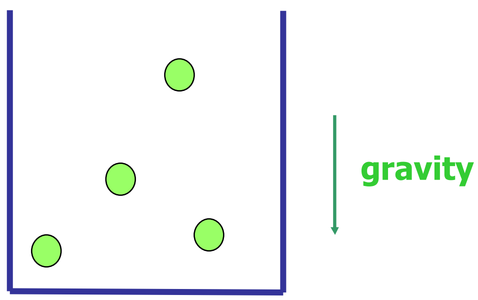
$PV/E-1=2\nu g(\nu)$

phase transition

at critical density

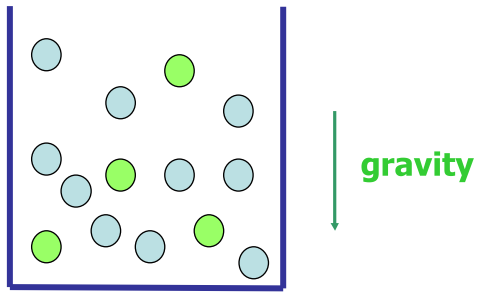
fluid, disordered

Elastic hard spheres in gravity



- **N particles**
- **Kinetic Energy**
- **What is the *density profile* ?**

Elastic hard spheres in gravity



- **N particles**
- **Kinetic Energy**
- **What is the *density profile* ?**

Elastic hard spheres in gravity

elastic steady state: $\frac{\partial}{\partial t} = 0 \qquad u_i = I = 0$

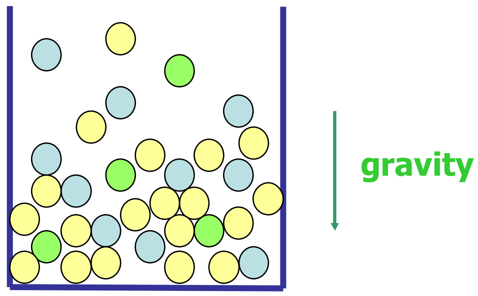
mass & energy conservation – OK

momentum balance:

$$0 = -\frac{\partial}{\partial x_i} P + \rho g_i$$

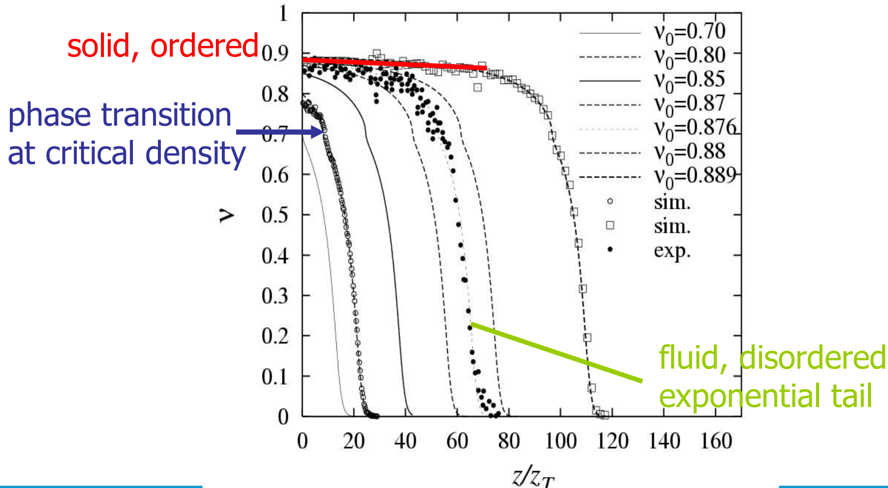
- **Pressure *P* *global equation of state***
- **Shear Stress** $\sigma_{ij}^{\mathrm{dev}} = 0$
- **Energy Dissipation Rate *I=0***

Elastic hard spheres in gravity

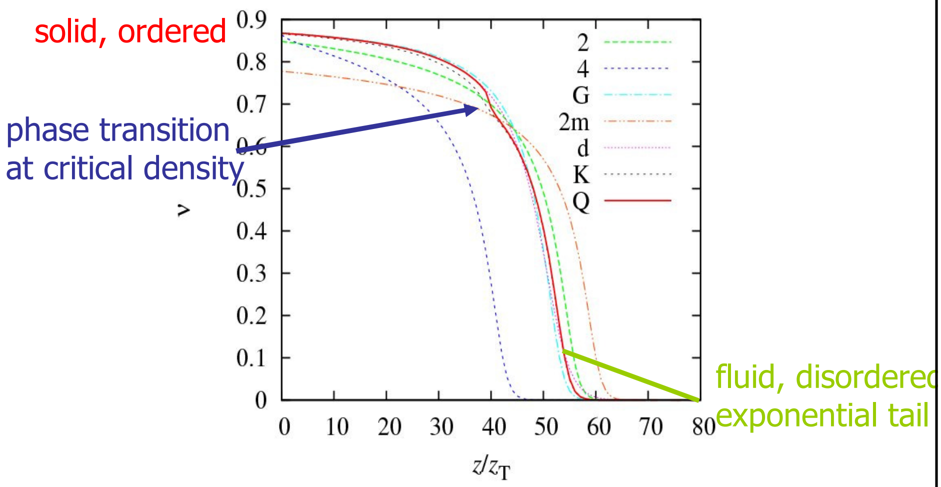


- **N particles**
- **Kinetic Energy**
- **What is the *density profile* ?**

Hard sphere gas in gravity



Hard sphere gas in gravity



Continuum theory

steady state …

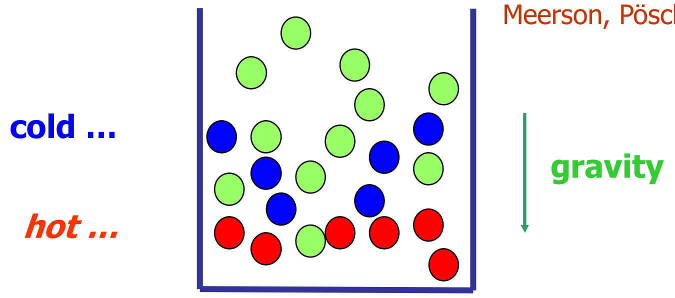
momentum conservation: $$0 = -\frac{\partial}{\partial x_i} P + \rho g_i$$

energy balance: $$0 = \frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho v^2\right) = -\frac{\partial}{\partial x_k}\left[-K \frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right] - I$$

- **Pressure *P***
- **Shear Stress** $\sigma_{ij}^{\text{dev}} = 0$
- **Energy Dissipation Rate *I***

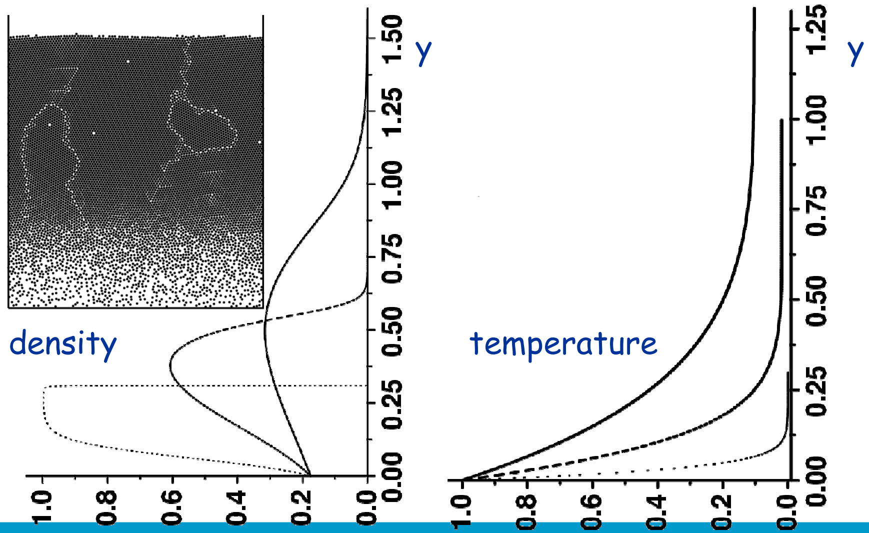
In-elastic hard spheres in gravity

Meerson, Pöschel, …, 2003



- **N particles**
- **Kinetic Energy – Input**
- **What are the *temperature* and *density profiles* ?**

Density inversion: Results from T. Pöschel and B. Meerson



Continuum theory

mass conservation:

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

momentum conservation:

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

energy balance:

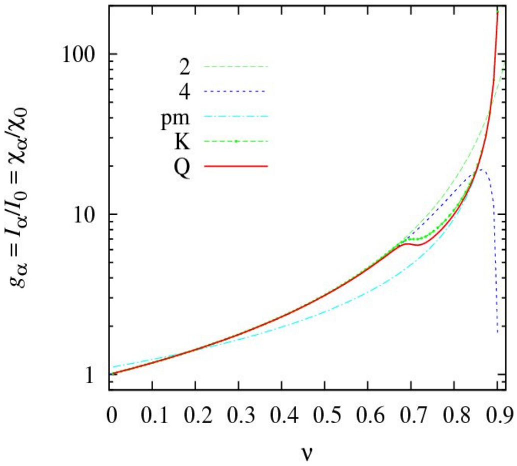
$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho u^2+\tfrac{1}{2}\rho v^2\right)= -\frac{\partial}{\partial x_k}\left[\rho u_k\left(\frac{P}{\rho}+\tfrac{1}{2}u^2+\tfrac{1}{2}v^2\right) -u_i\sigma_{ik}^{\mathrm{dev}}-K\frac{\partial}{\partial x_k}\left(\tfrac{1}{2}\rho v^2\right)\right]+\rho u_i g_i-I$$

- **Pressure P**
- **Shear Stress $\sigma_{ij}^{\mathrm{dev}}$**
- **Energy Dissipation Rate I**

… dissipation rate

$$I=I\left(g_{2a}(\nu)\right)$$

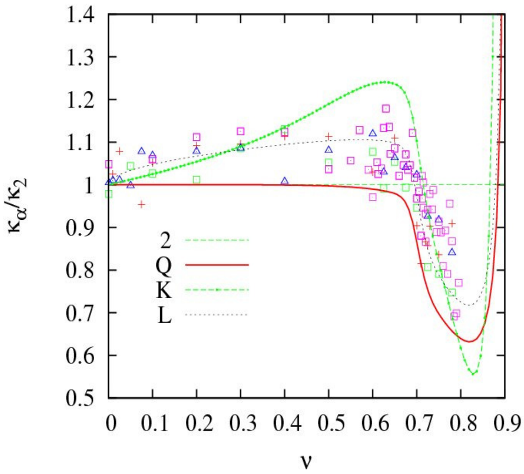
… dissipation rate



… heat-conductivity

$$K = K\left(g_{2a}\left(\nu\right)\right)$$

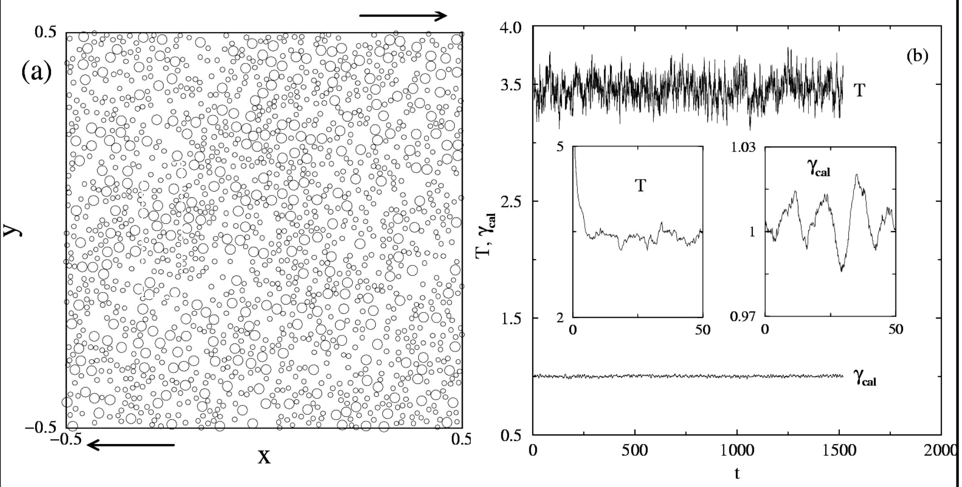
… heat-conductivity



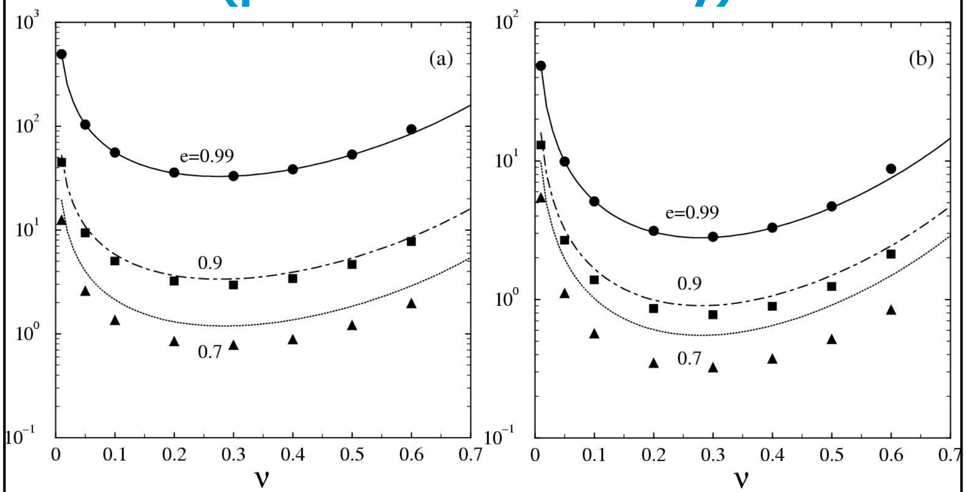
… shear-viscosity

$$\eta = \eta\left(g_{2a}(\nu)\right)?$$

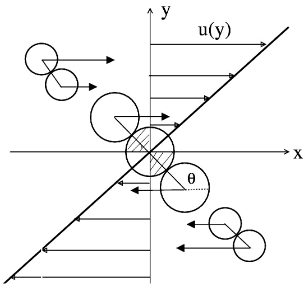
Shear (energy and rate)

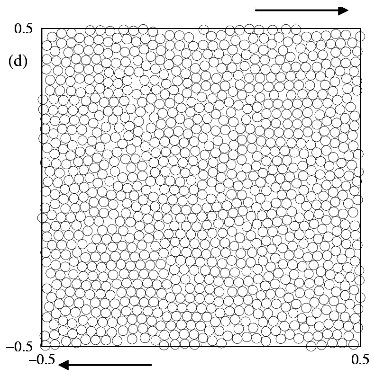


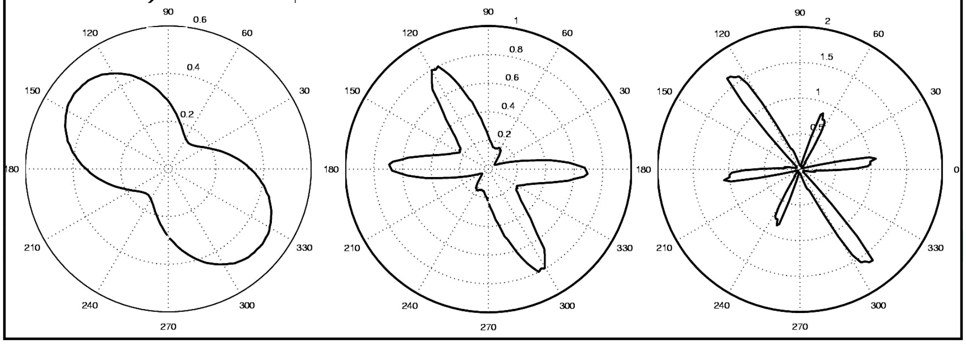
Shear (pressure and viscosity)



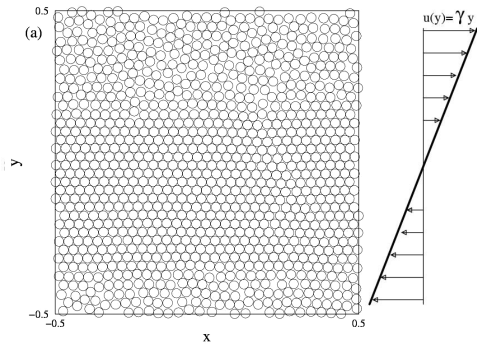
Structure formation

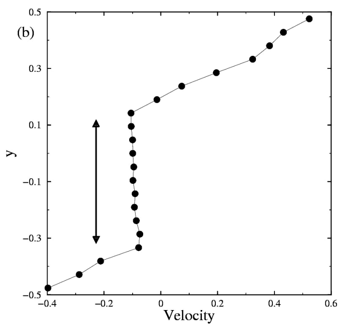






Structure formation

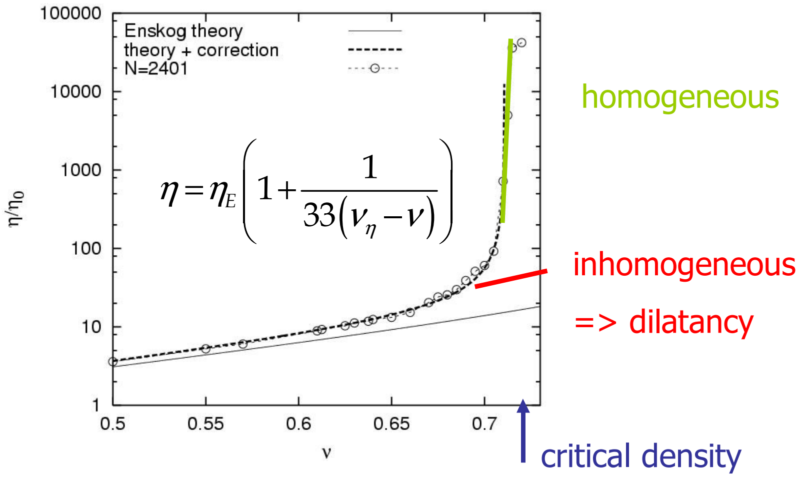




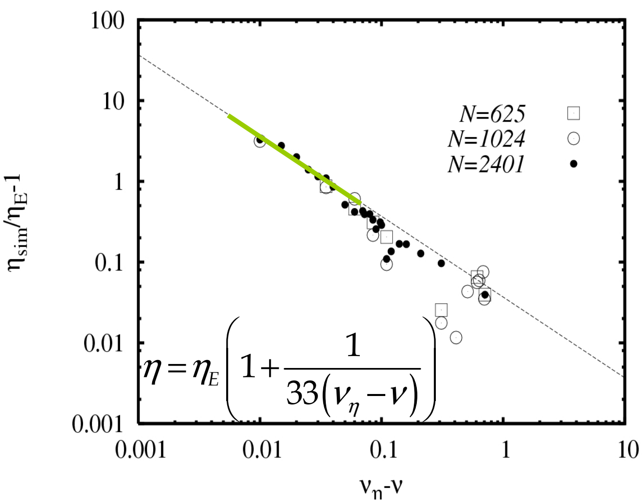
Low density -> linear velocity profile

High density -> shear localization

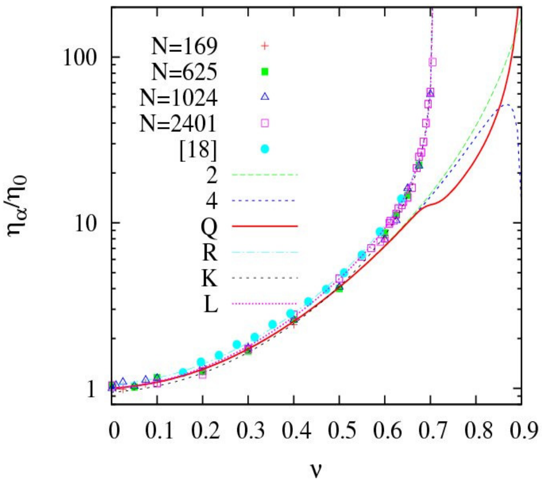
Shear (viscosity at high density)



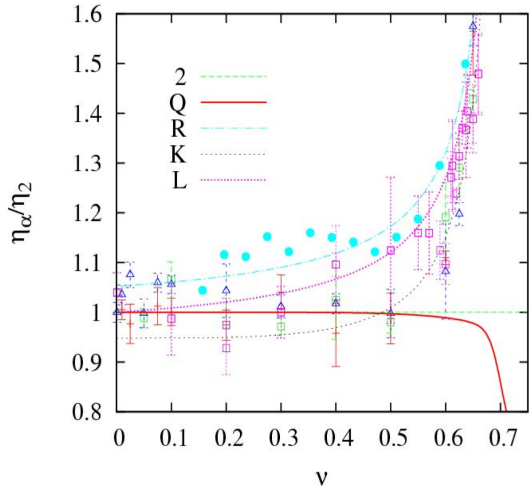
Shear viscosity divergence



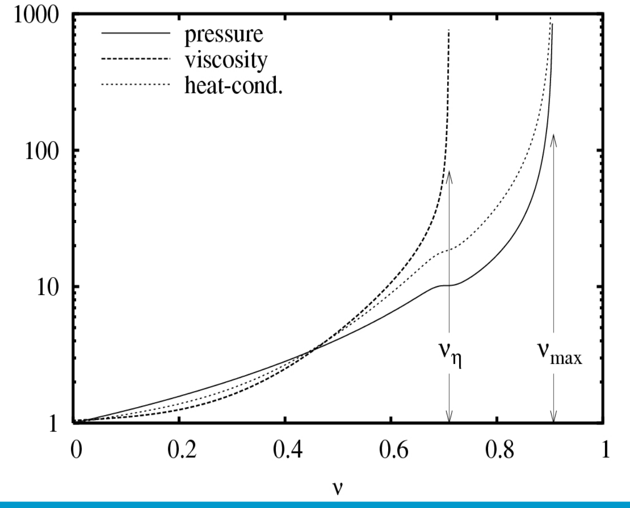
shear “viscosity” (2D)



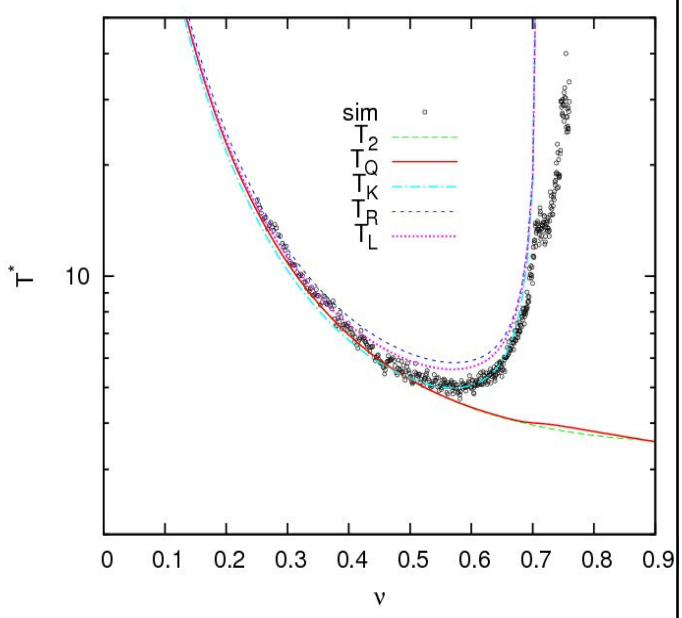
shear “viscosity” (2D)



Global equations of state (2D)



Sheared systems r=0.998



Continuum theory

mass conservation:

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

momentum conservation:

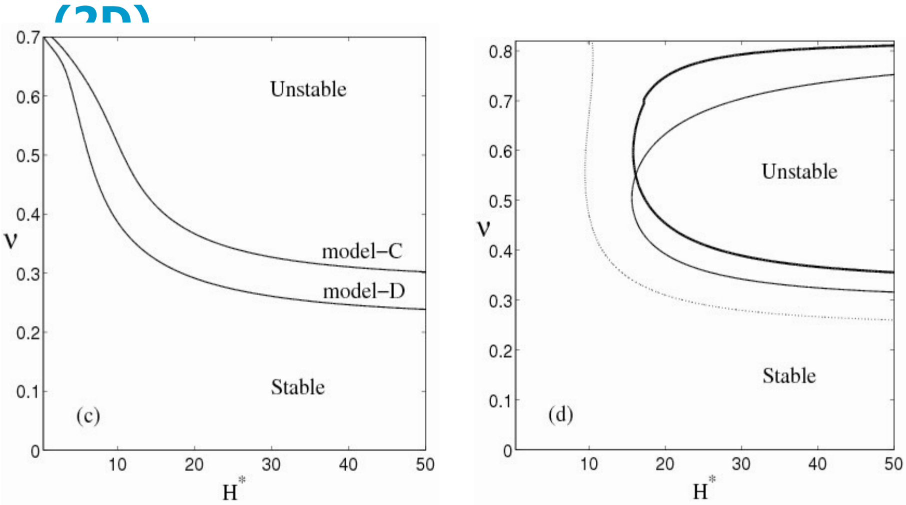
$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_k}(\rho u_i u_k) = -\frac{\partial}{\partial x_i}P + \frac{\partial}{\partial x_j}\sigma_{ij}^{\mathrm{dev}} + \rho g_i$$

energy balance:

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

- **Pressure P**
- **Shear Stress $\sigma_{ij}^{\mathrm{dev}}$**
- **Energy Dissipation Rate I**

Sheared systems – linear stability (2D)



Shukla, Alam, Luding, 2008

Continuum theory

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energy balance:

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

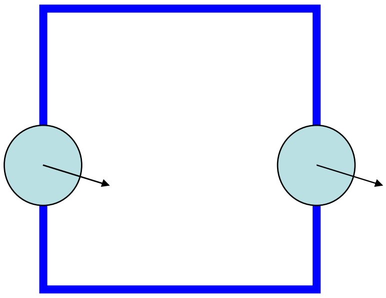
- **Pressure *P***
- **Shear Stress** σ_{ij}^{dev}
- **Energy Dissipation Rate *I***

Summary (1)

- Density profiles – simulations and experiment
  - Continuum: Global equations of state
- Theory and simulation agree very well for large *r*
  - Homogeneous and sheared
- *Open issues:*
  - Dense (inhomogeneous) systems
  - Anisotropy, micro-structure, …
  - Realistic boundary conditions, …
  - Experimental validation, …

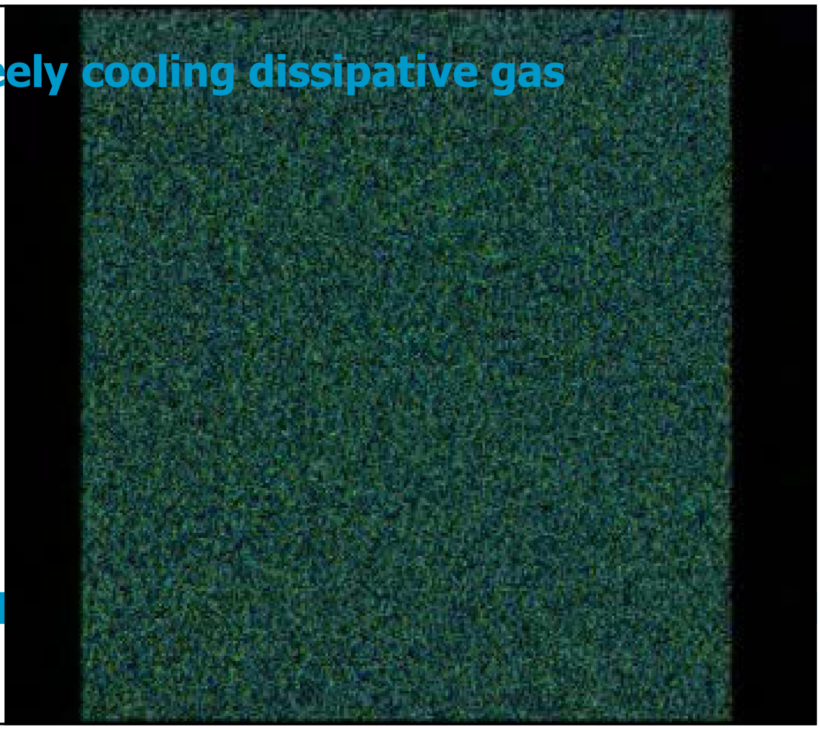
Dissipative hard spheres - no friction

simulate *N* particles
in a peridoc box



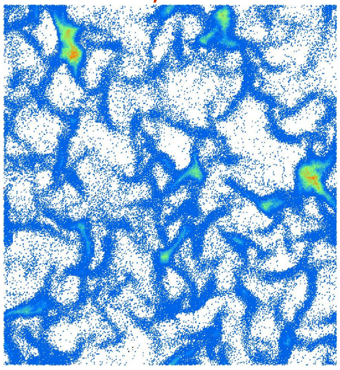
Freely cooling dissipative gas

2D



How to understand clustering ?

Goldhirsch, Zanetti 1993, …



- Higher density
- More dissipation
- Lower Pressure
- etc.

… is that all ?

… equations of state for all densities

Freely cooling system

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

mass & momentum conservation – OK

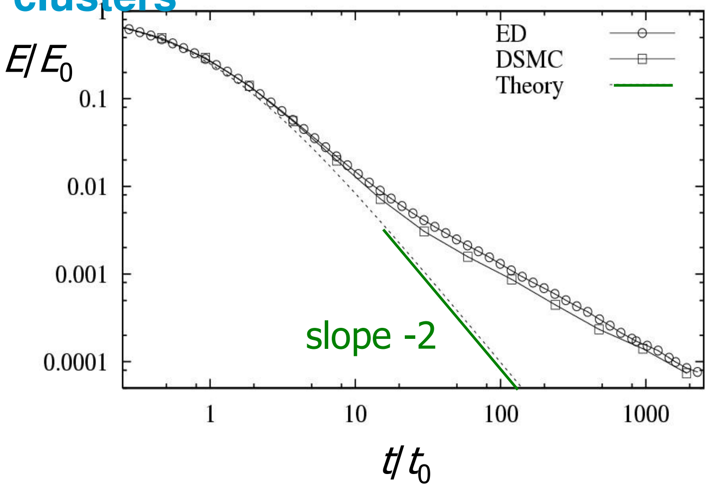
energy balance: $\frac{\partial}{\partial t}\left(\frac{1}{2}\rho v^2\right) = -I \qquad I \propto \rho\left(1-r^2\right)v^3$

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 => clusters



Static vs. dynamic
another order parameter?

TC model allows to define

- "potential" energy
- "static" contacts

beyond the limits of
hard sphere model validity

$$\tau_c := \frac{t_c}{t_n} > 1: \quad \text{static}$$

$$\tau_c := \frac{t_c}{t_n} < 1: \quad \text{collisional}$$

$+\text{dynamic}$

Continuum theory

mass conservation:

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

momentum conservation:

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

energy balance:

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

- **Pressure P**
- **Shear Stress $\sigma_{ij}^{\mathrm{dev}}$**
- **Energy Dissipation Rate I**

Summary

From dilute to dense systems

- **Pressure** (equation of state for all densities 2D)
  - Phase Transition (Disorder-Order)
- **Shear viscosity - early divergence => jamming**
- **Heat conductivity weak difference from pressure**
- **Energy Dissipation - delayed at high density due to multi-particle contacts**

Summary & Conclusion

From dilute to dense systems

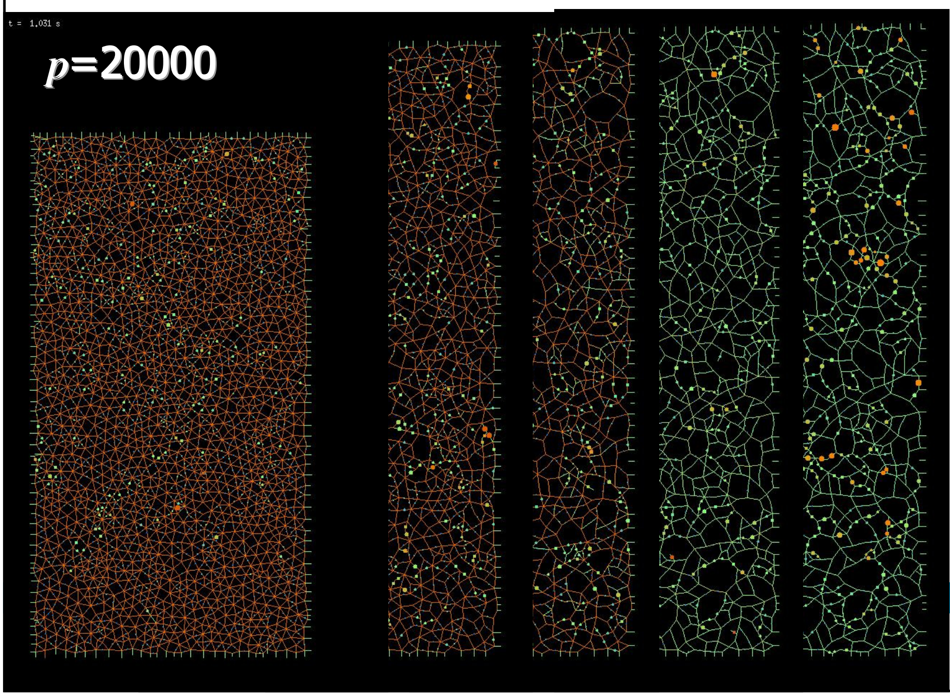
- **Pressure** (equation of state for all densities 2D)
  - Phase Transition (Disorder-Order)
- **Shear viscosity - early divergence => jamming**
- **Heat conductivity weak difference from pressure**
- **Energy Dissipation - delayed at high density due to multi-particle contacts**
- **Correct the EQS, dissipation, transport-coeff. for QUANTITATIVE predictions using continuum theory & solvers**

Granular fluids & solids …

- **compressibility? / dilatancy?**
- **MohrCoulomb-like yield stress?**
- **shear viscosity?**
- **inhomogeneity? (force-chains)**
- **(almost always) an-isotropy?**
- **micro-polar effects (rotations) …**

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

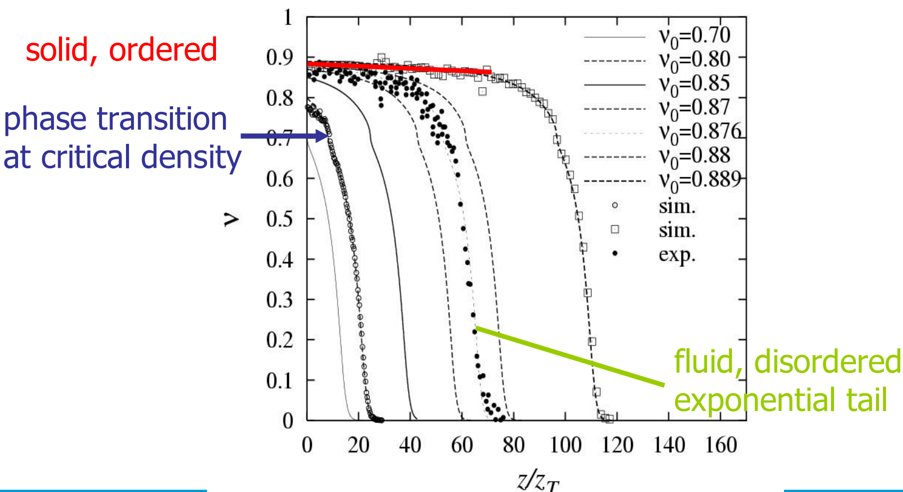


Granular flow …

- **compressibility? / dilatancy?**
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

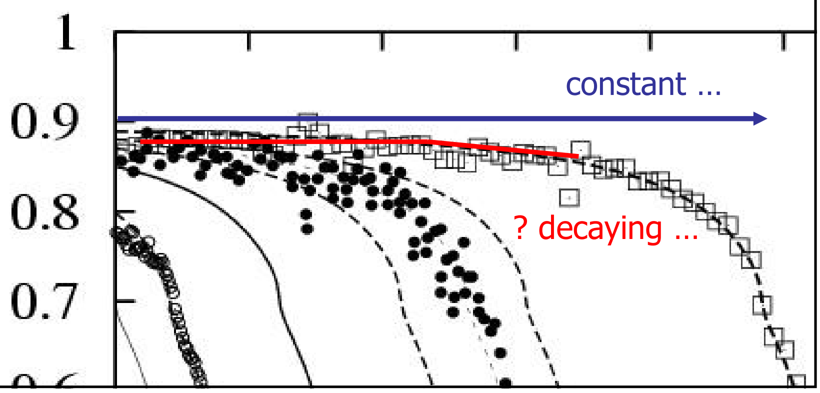
VERY small changes in density ⇔
VERY LARGE changes in pressure!

Hard sphere gas in gravity



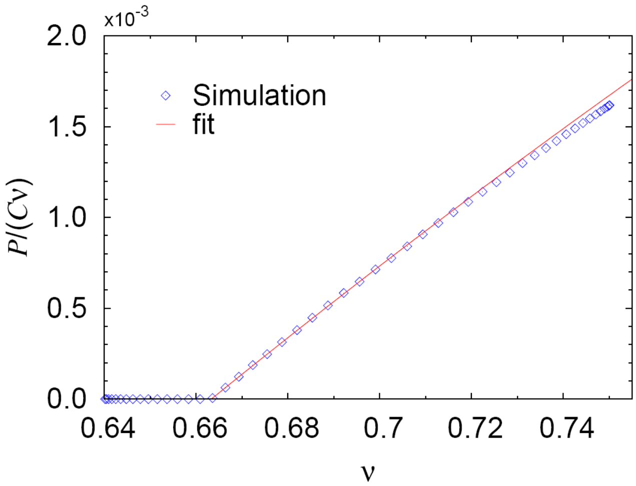
Constant density regime?
… don’t trust it – look closer!

… constant density? … check errors …



Pressure $\frac{P}{C\nu} = P_{\text{ref}} \log\left(\frac{\nu}{\nu_c}\right)$

$$e = \frac{1}{\nu} - 1$$



N = 10000

$w = 3$

P_{ref} scales w

$\nu_c = 0.6624$

Granular flow …

- compressible!!! / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

➢ **DO NOT assume constant density**
➢ **consider contact-number*density**

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

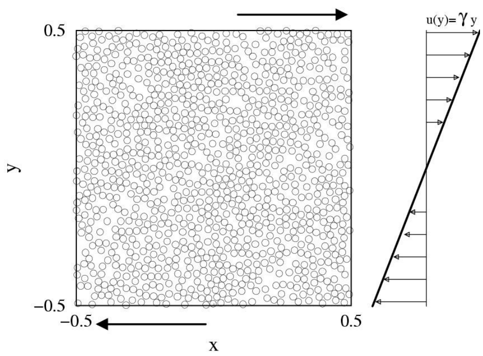
➢ **later …**

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear **viscosity?**
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

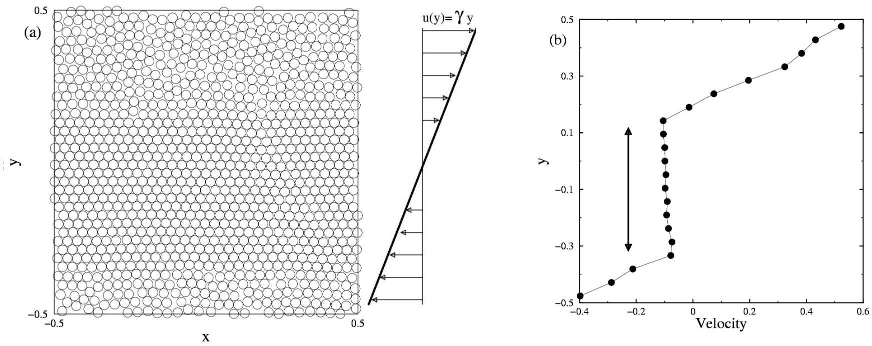
Shear -> Viscosity

$$\frac{|\tau|}{\dot{\gamma}} \quad \text{vs.} \quad I = \frac{\dot{\gamma} d_0}{\sqrt{p/\rho_0}}$$



Low density -> linear velocity profile

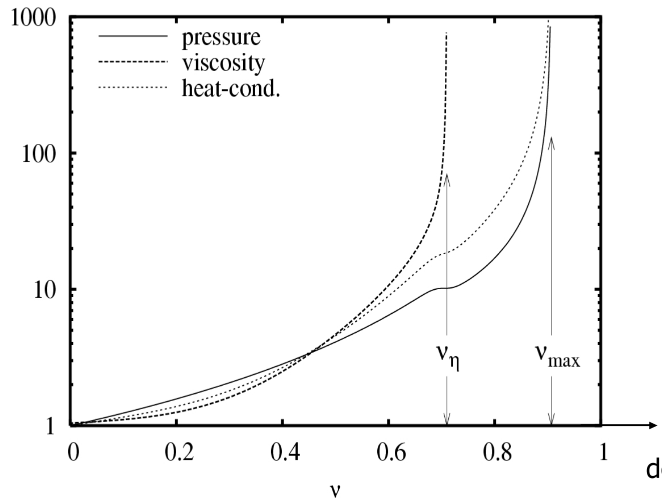
Shear -> Localisation/Shear-Band



Low density -> linear velocity profile

High density -> shear localization

Monodisperse, almost elastic ... (2D hom.)



density

RG Rojo, SL, JJ Brey, PRE 2006 and E Khain, PRE, 2007,9

Granular flow …

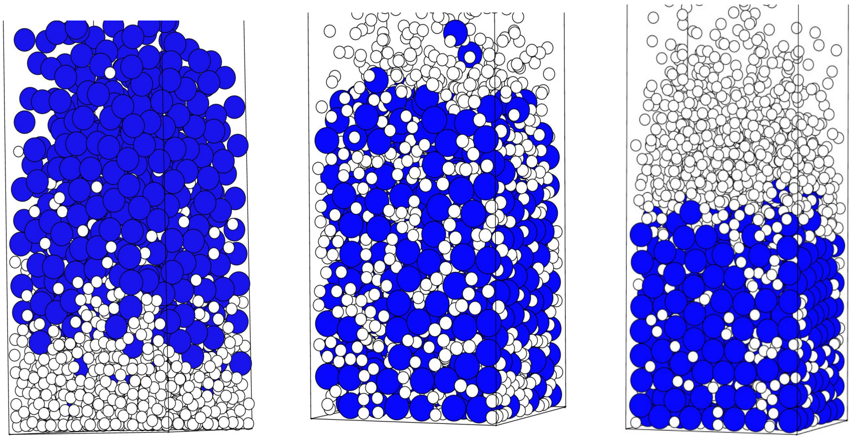
- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

➢ **INTERESTING … for higher densities**
➢ **TRICKY in presence of anisotropy (later)**

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (segregation)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

Segregation – Mixing – Reverse segregation

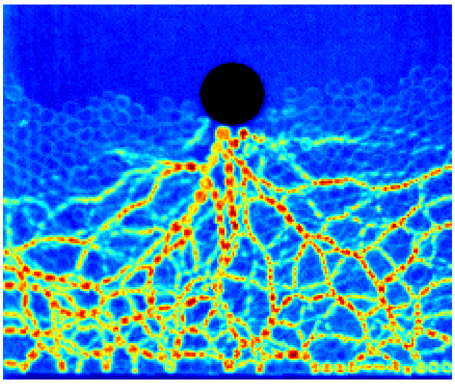


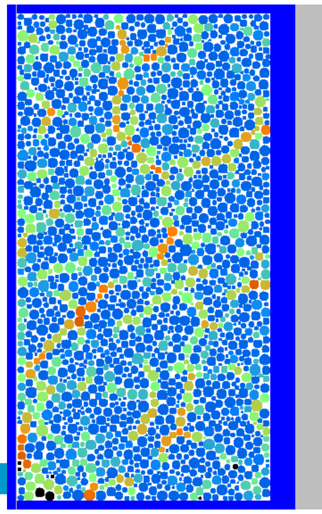
PV Quinn, D Hong, SL, PRL 2001

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

Force-chains
experiments - simulations





Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (clustering)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (shear-bands)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

➢ **HOW TO AVOID inhomogeneity?**
➢ **WHAT TO DO if inhomogeneous?**

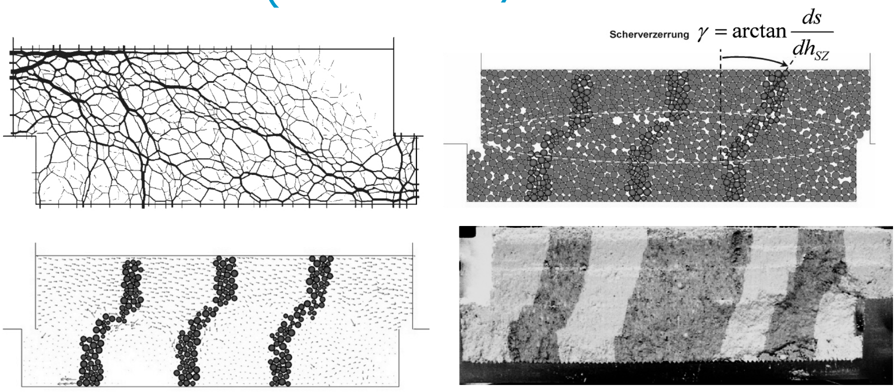
Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (shear-bands)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

➢ **HOW TO AVOID inhomogeneity?**
➢ **WHAT TO DO if inhomogeneous?**

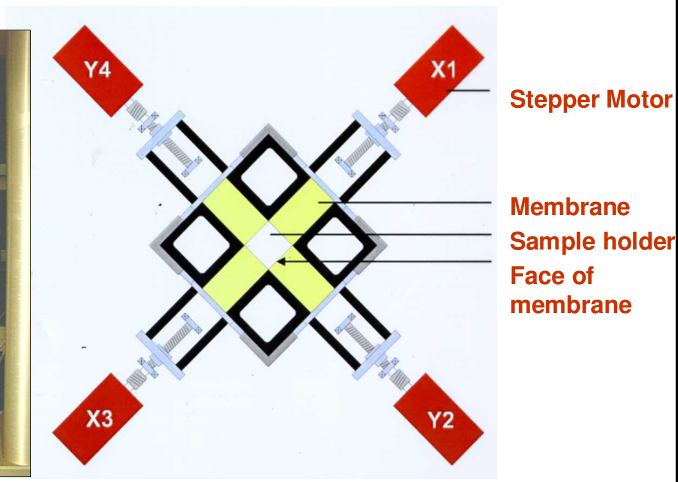
➢ **Choose a "good" experiment**

Jenike cell (sim. PFC2D)



Standard experiments -> inhomogeneous:
Cohesive, fine powders, (Tomas, Magdeburg)

3D shear experiments



Biaxial box set-up

- Top wall: strain controlled

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

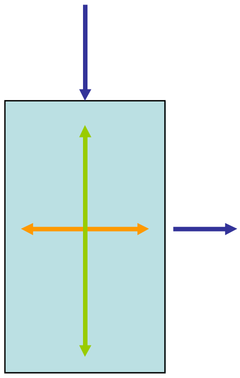
- Right wall: stress controlled

$$dp, V, \sigma_{xx} = \text{const.}$$

- Evolution with time … ?

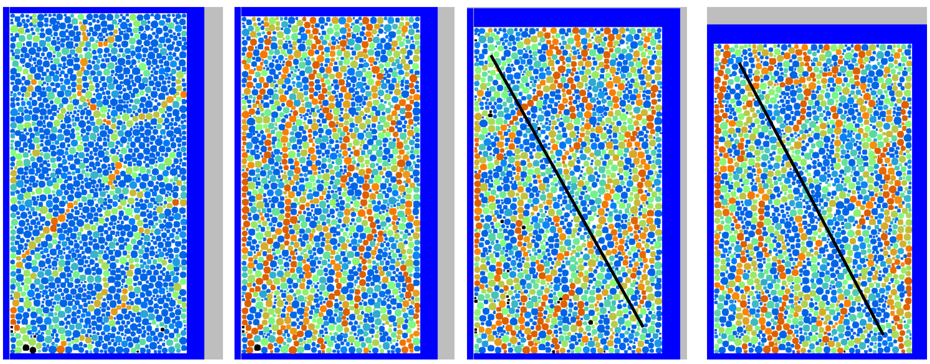
- ADVANTAGES!!!

  … but also inhomogeneous …



Simulation results (closer look)

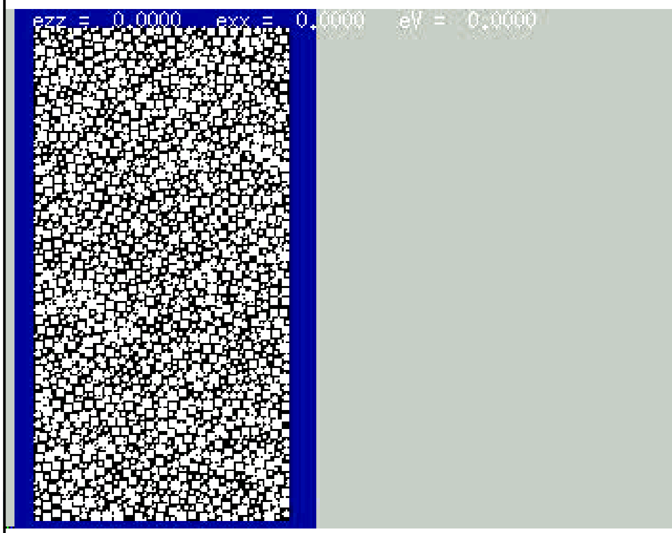
ε_{zz}=0.0% ε_{zz}=1.1% ε_{zz}=4.2% ε_{zz}=9.1%



Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- **(almost always) an-isotropy?**
- micro-polar effects (rotations) …

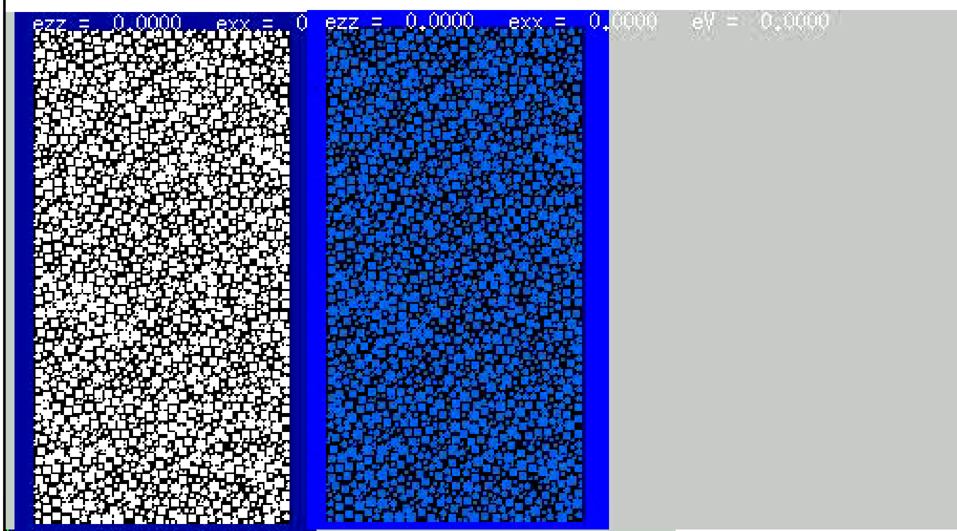
Bi-axial box (stress chains)



Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (shear-band)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

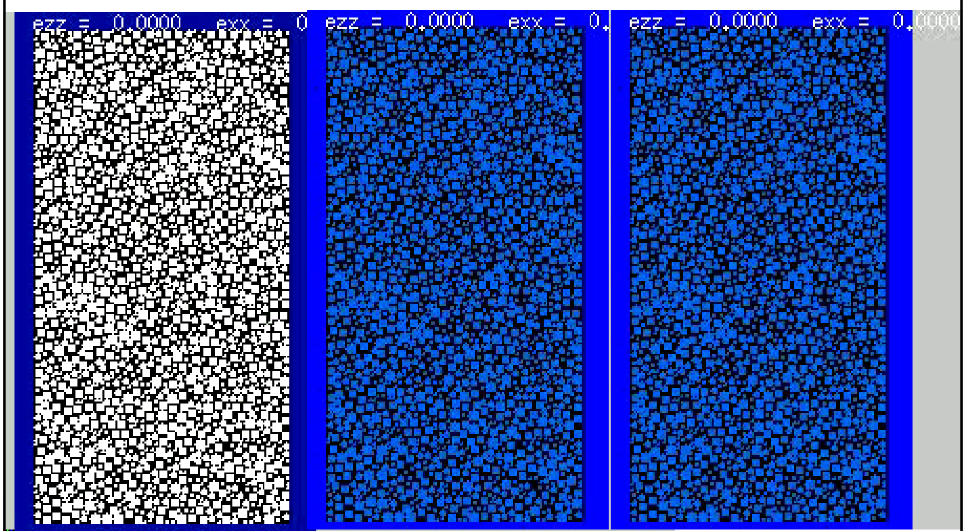
Bi-axial box (kinetic energy)



Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- **micro-polar effects (rotations) …**

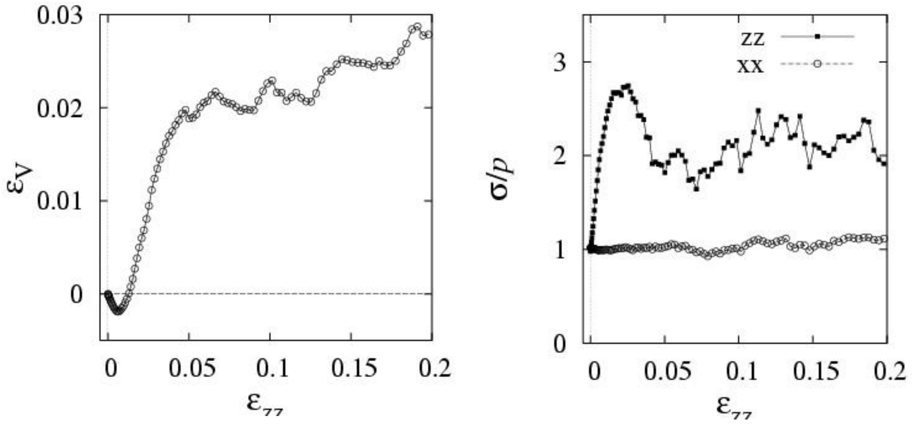
Bi-axial box (rotations)



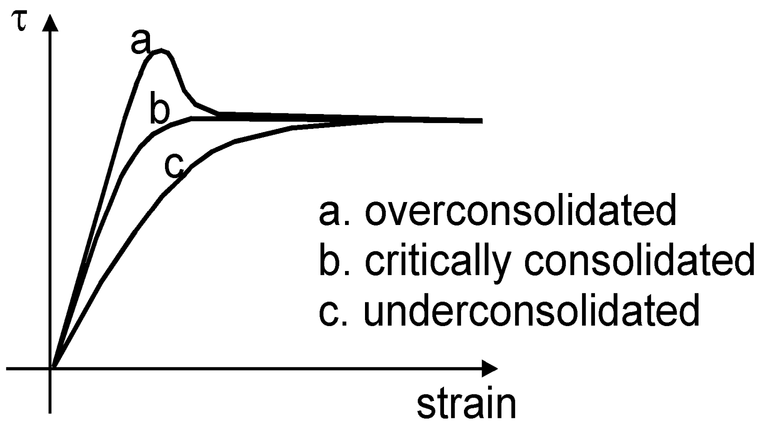
Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

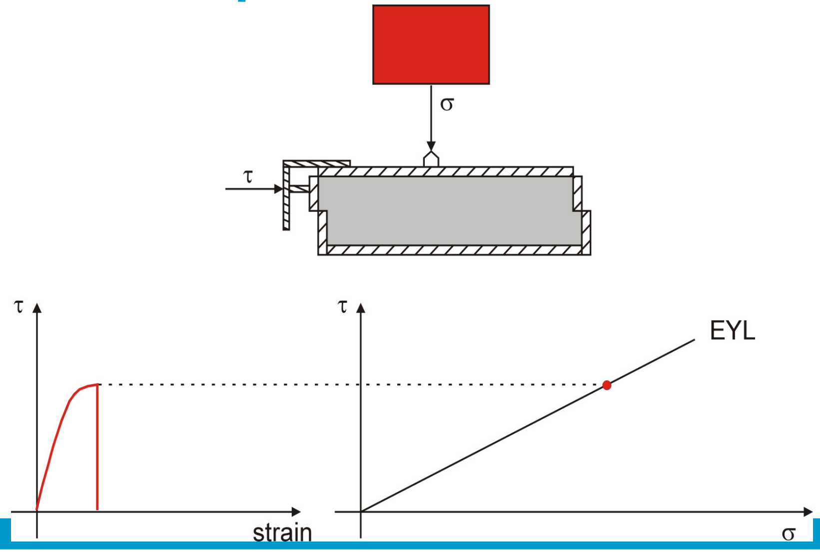
Bi-axial compression with p_x=const.



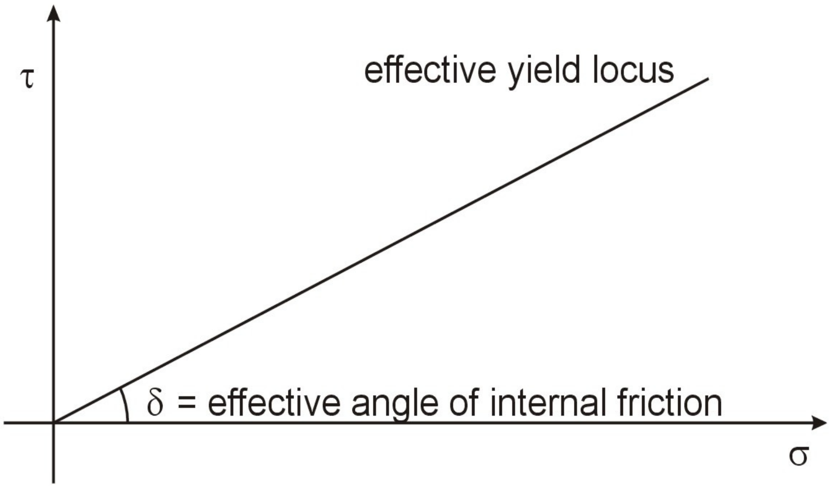
Microscopic interpretation: memory?



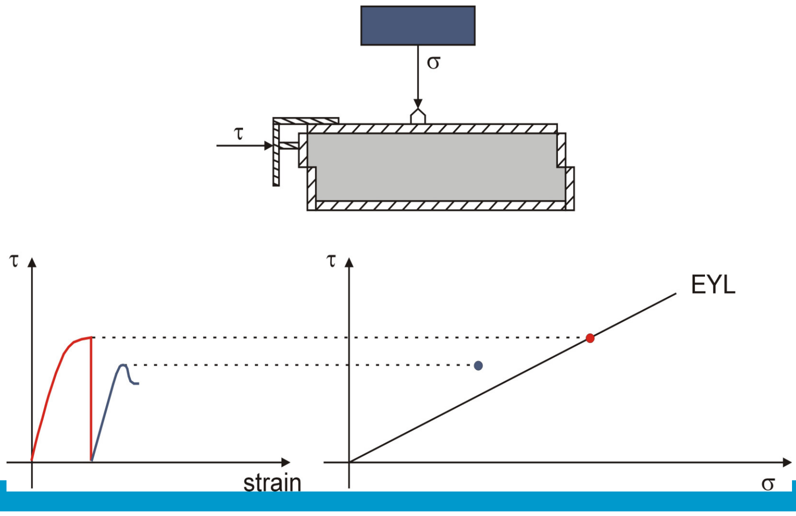
Yield locus procedure 1



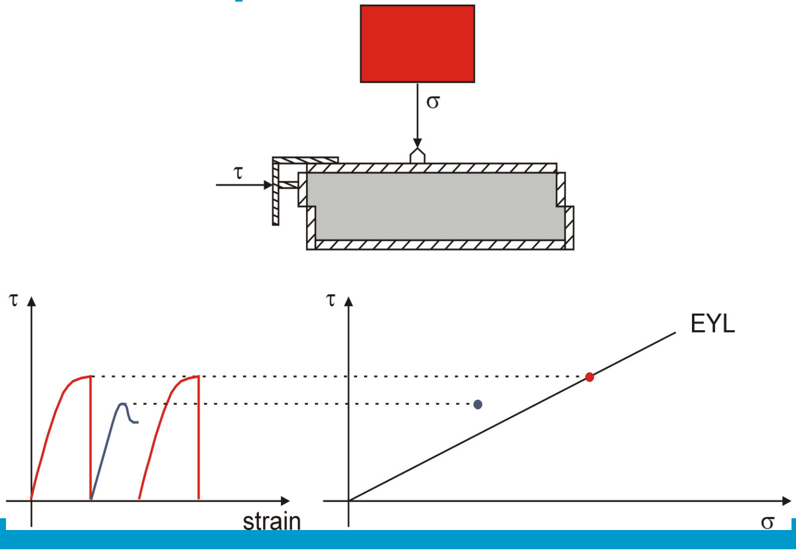
Effective yield locus



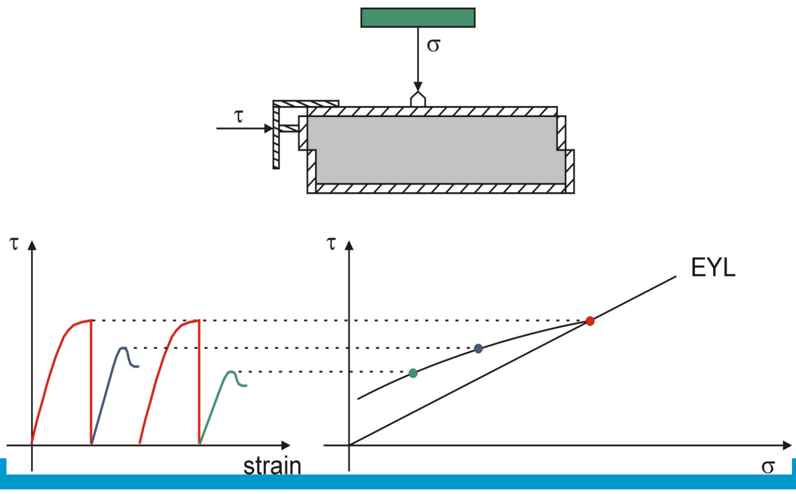
Yield locus procedure 2



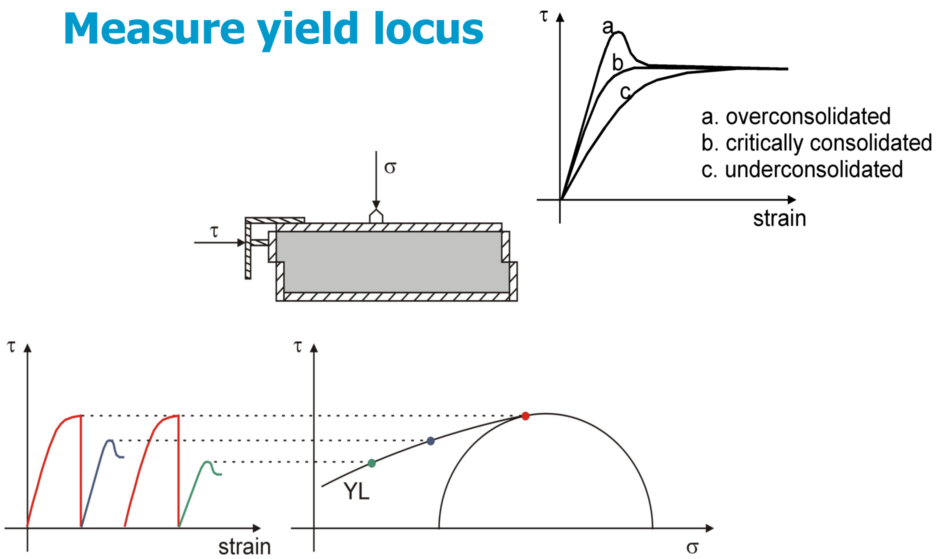
Yield locus procedure 3



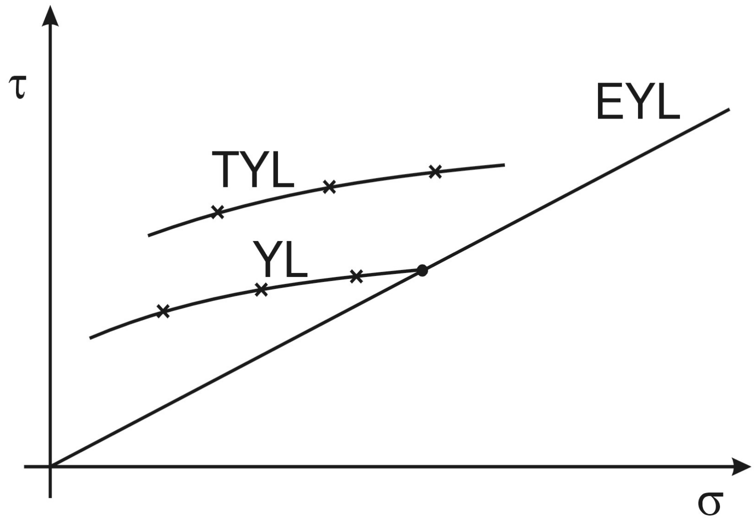
Yield locus procedure 4



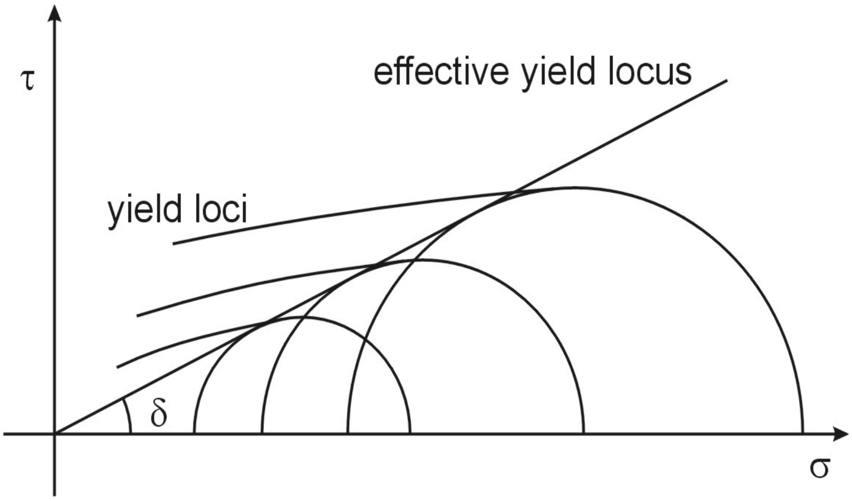
Measure yield locus



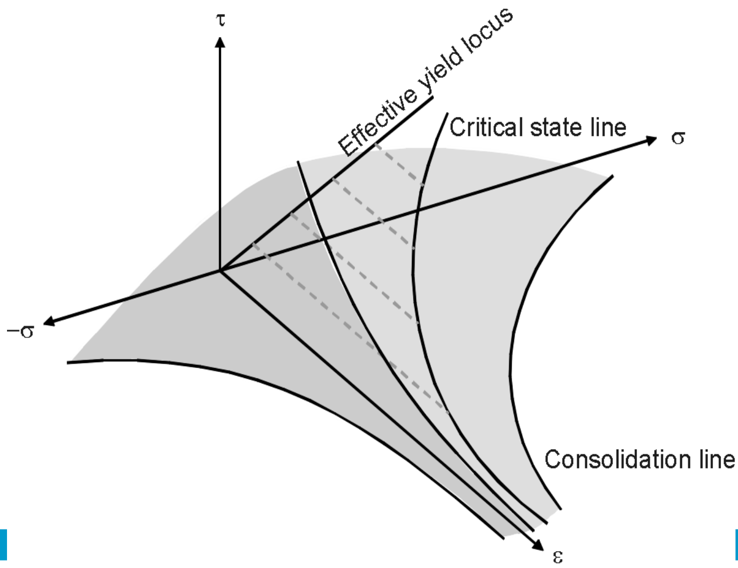
Time yield locus



Yield loci

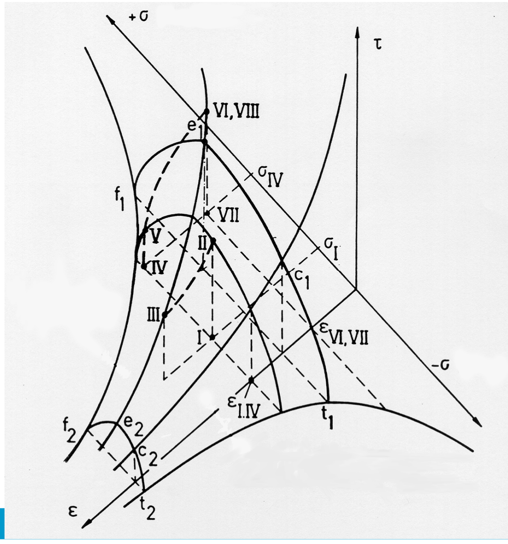


Hvorslev diagram (-50 years) <-> jamming diagram

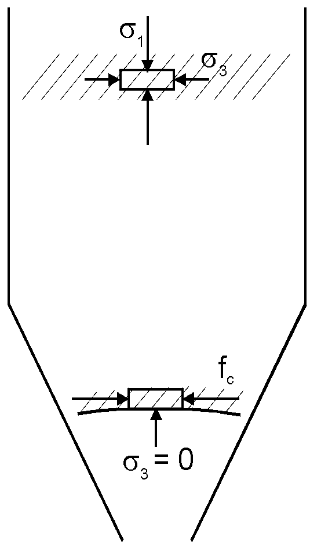


porosity = 1 - volume fraction

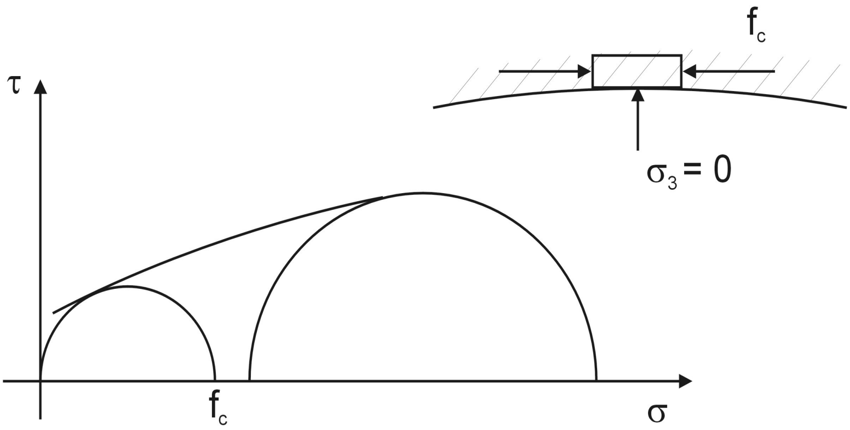
Consolidation and Failure Surfaces



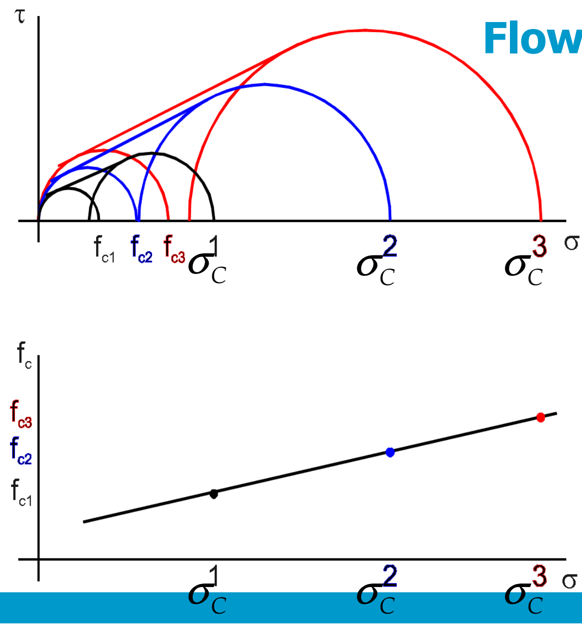
Flow Function (ff)



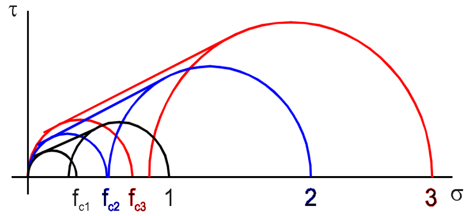
Unconfined yield strength

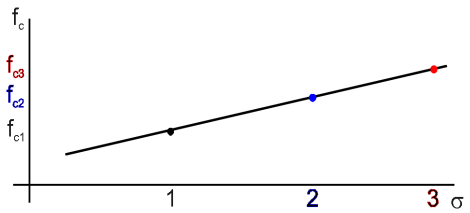


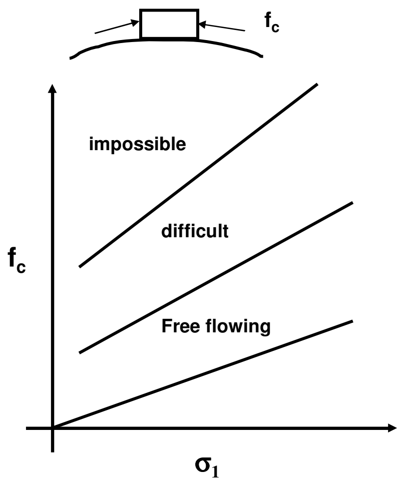
Flow Function (ff)



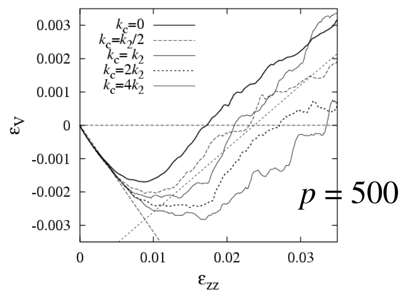
Flow behavior

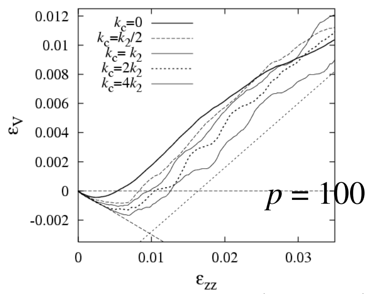






Material parameters





Initial Compression:

$$\frac{\varepsilon_v}{\varepsilon_{zz}} = \tan^{-1}(1-2\nu)$$

Poisson-ratio: $\nu \approx 0.66$

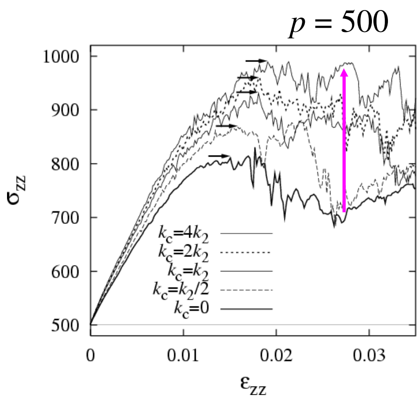
Dilatancy: $d' = \tan^{-1}\left(\frac{2\sin\psi}{1-\sin\psi}\right)$

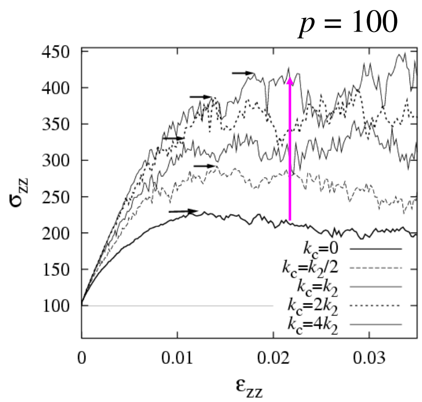
Dilatancy Angle:

$\psi \approx 0.088$ **for** $p = 500$

$\psi \approx 0.190$ **for** $p = 100$

Modulus and yield stress cohesion

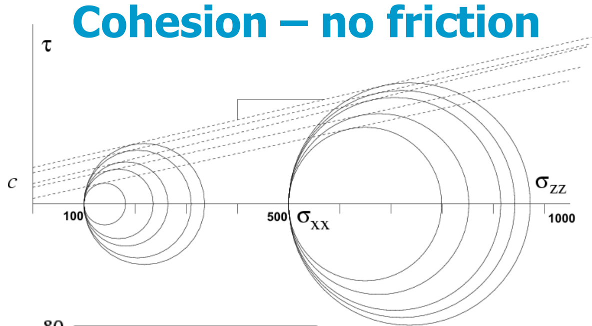




Modulus
(initial slope)

Yield Stress ....
(peak value)

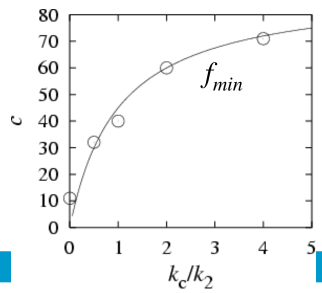
Cohesion – no friction



$k_c / k_2 = 0, 1/2, 1, 2, \text{ and } 4$

geometrical friction angle

$\phi \approx 13^\circ$

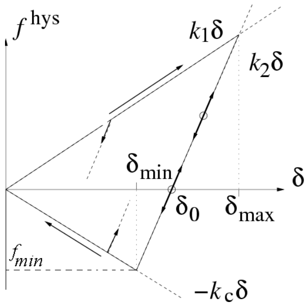


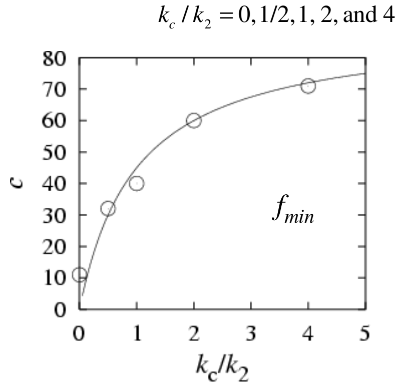
macro cohesion

$c = 1.8\times10^{-3}\,\frac{1-k_1/k_2}{1+k_2/k_c}$

k_c/k_2	p_x	σ_{zz}	p_x	σ_{zz}	c
0	100	183	500	798	11
½	100	234	500	853	32
1	100	264	500	915	40
2	100	310	500	941	60
4	100	336	500	972	71

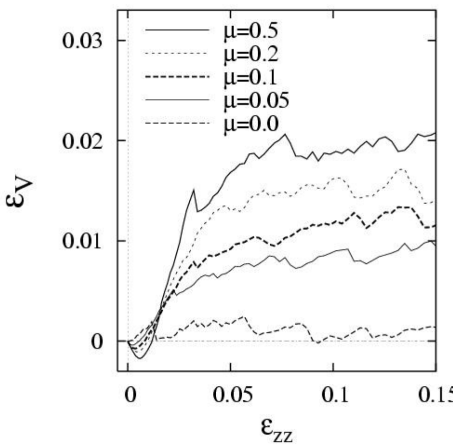
Micro-macro for cohesion

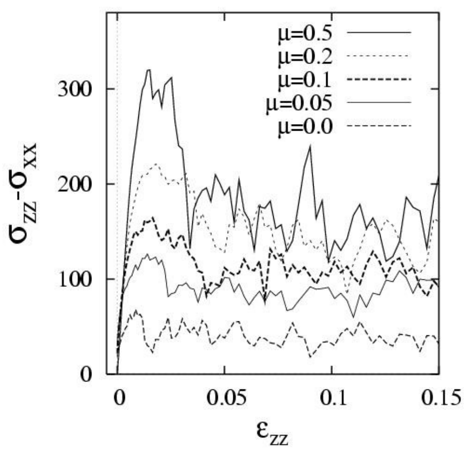




micro adhesion: f_{min} macro cohesion $c = c_0 \dfrac{1 - k_1/k_2}{1 + k_2/k_c}$

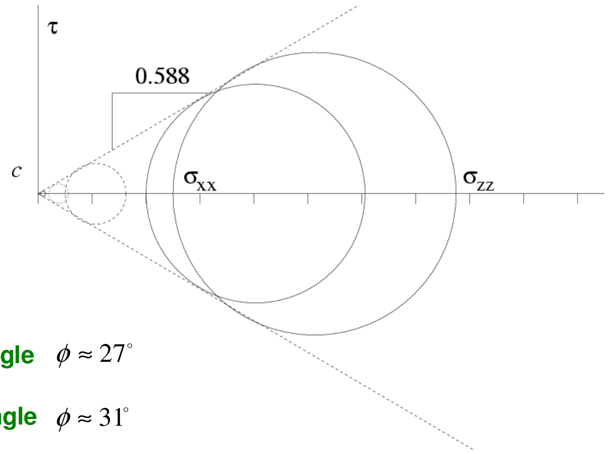
Bi-axial: p_x=200 – varying friction





Friction – no cohesion

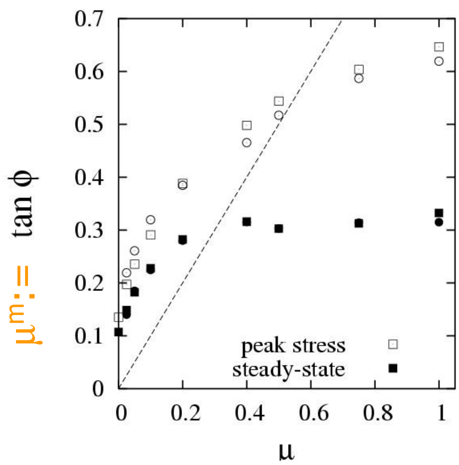
$k_c = 0$ and $\mu = 0.5$



Internal friction angle $\phi \approx 27^\circ$

Total friction angle $\phi \approx 31^\circ$

Micro-macro for friction



prepared μ=0

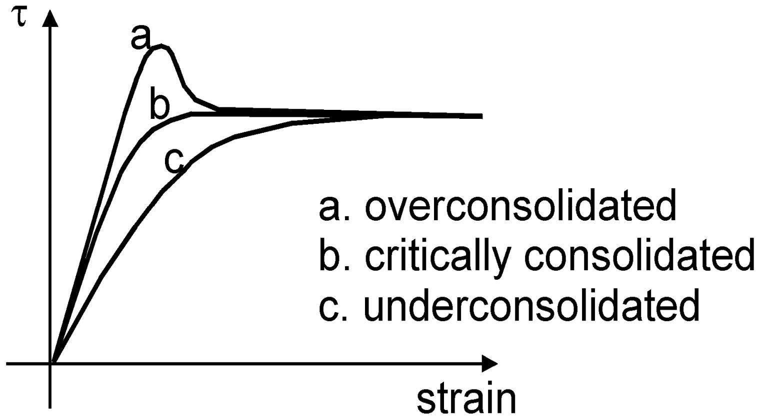
prepared μ=0.5

steady-state shear

micro contact-friction μ macro friction-angle ϕ

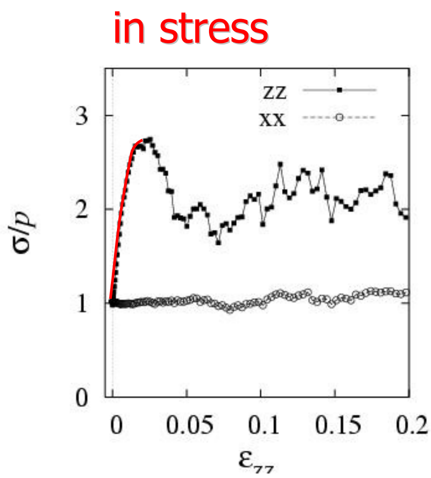
NOTE: each point = 5-10 simulations

Microscopic interpretation: memory?



An-isotropy

How to find a constitutive law?

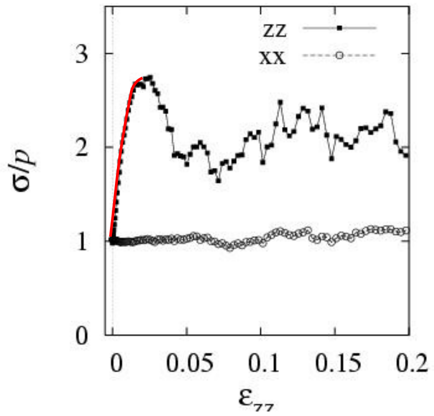


An-isotropy (Stress)

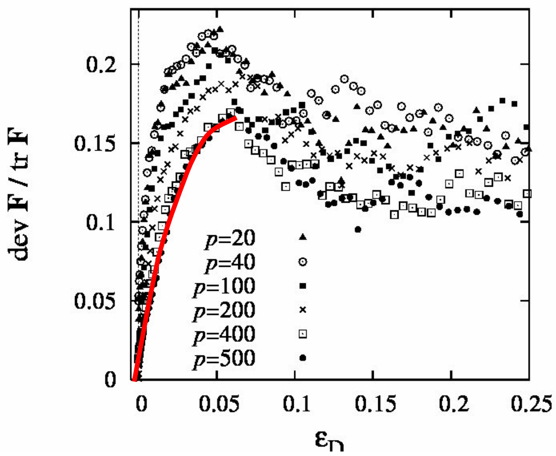
$$1 - s_D / s_{\max} = \exp\left(-\beta_s \varepsilon_D\right)$$

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

in stress



Fabric



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 – scalar

(in the biaxial box eigen-system)

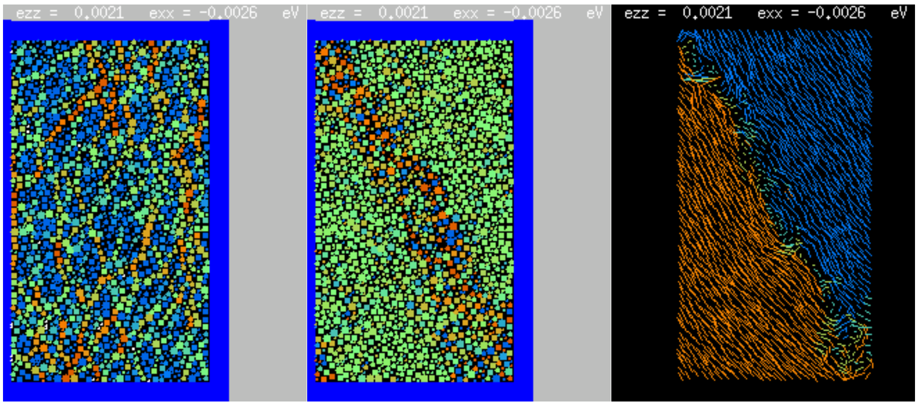
$$\delta\sigma_V = E\varepsilon_V + A\varepsilon_D$$

$$\delta\sigma_D = A\varepsilon_V + B\varepsilon_D$$

Global average vs. Local average

- Global
  - \+ Experimentally accessible data
  - \- Wall effects
  - \- Averaging over inhomogeneities
- Local
  - \- Difficult to compare to experiment
  - \+ Averages away from the walls
  - \+ Average over `similar' volume elements

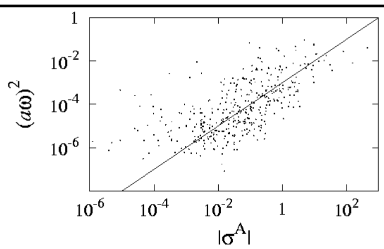
Micro informations: shear bands

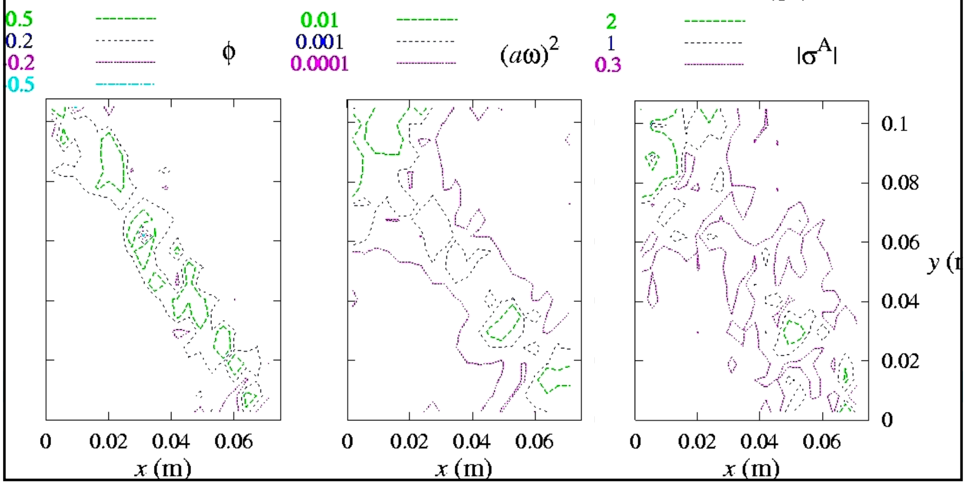


potential energy rotations displacements

Rotations (local)

Direction, amplitude,
anti-symmetric (!) stress



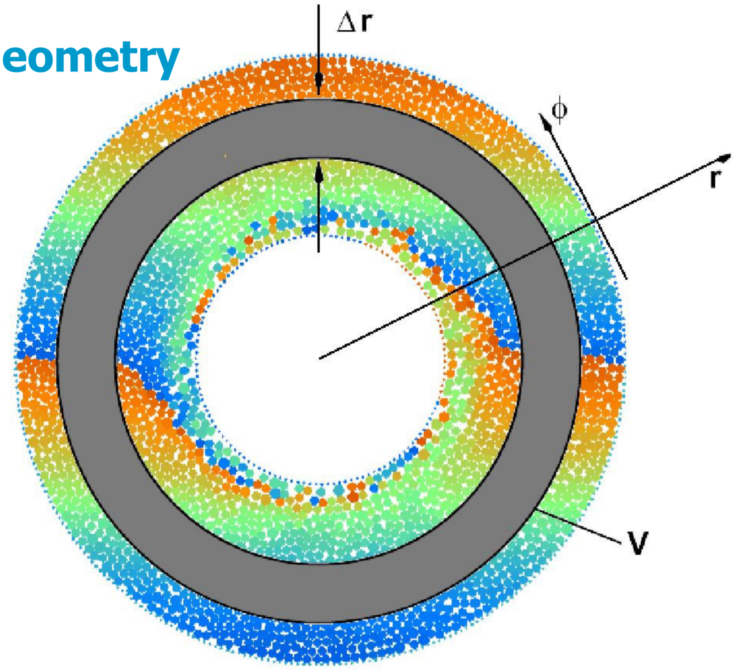


Summary micro-macro GLOBAL

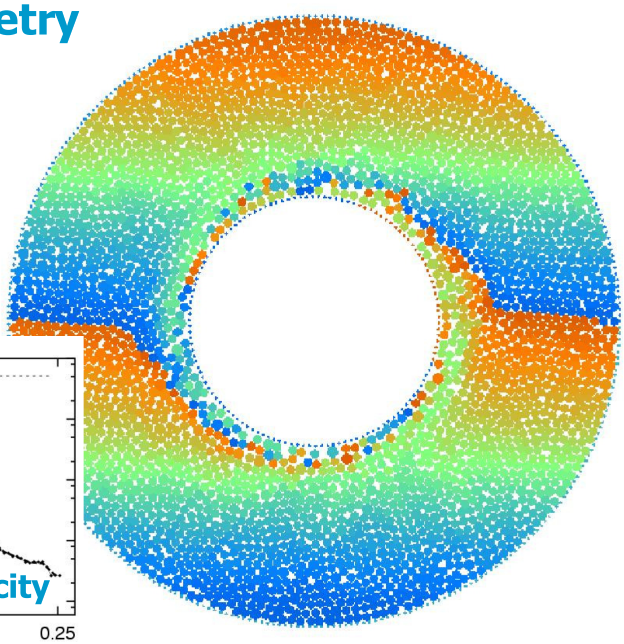
- Micro-/Macro-Flow Rheology
  - micro-adhesion … macro-cohesion
  - micro-contact-friction … macro-friction-angle
- Non-Newtonian Rheology (Anisotropy?, Micro-polar?)

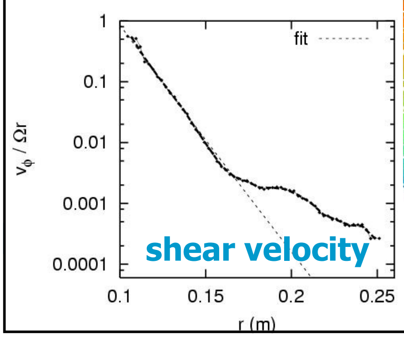
- **Does global averaging make sense anyway?**

Ring geometry



Ring geometry 2D





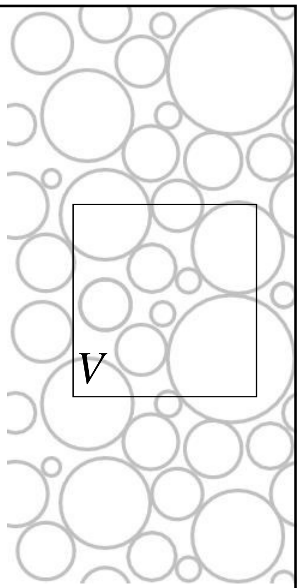
Averaging Formalism

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

Any quantity:

$$Q^p$$

In averaging volume: V

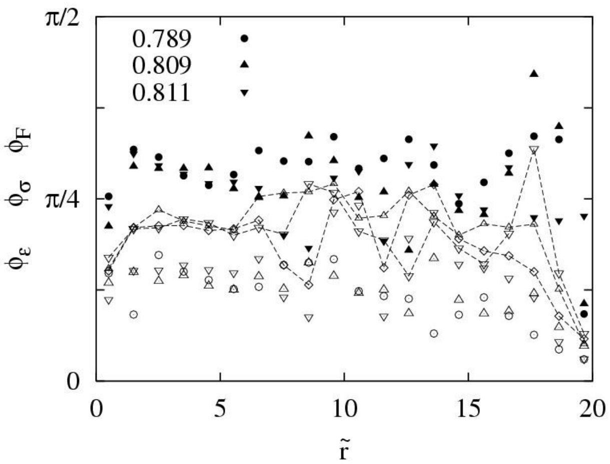


... simple or advanced ...

Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

Anisotropy –> non-colinearity !!!

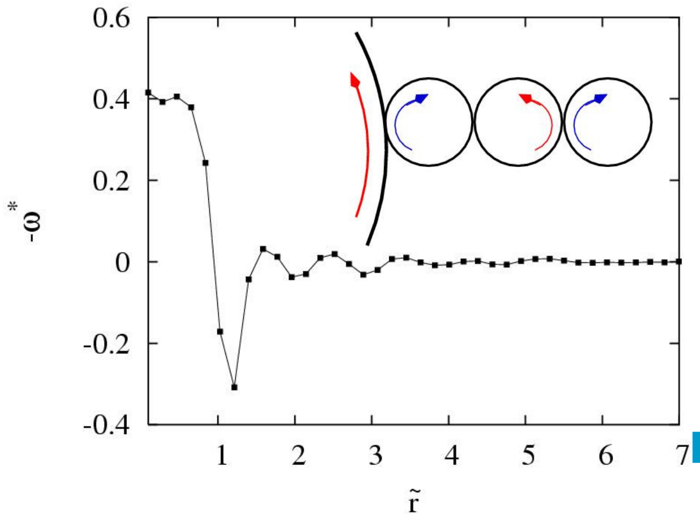


Granular flow …

- compressibility? / dilatancy?
- MohrCoulomb-like yield stress?
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- **micro-polar effects (rotations) …**

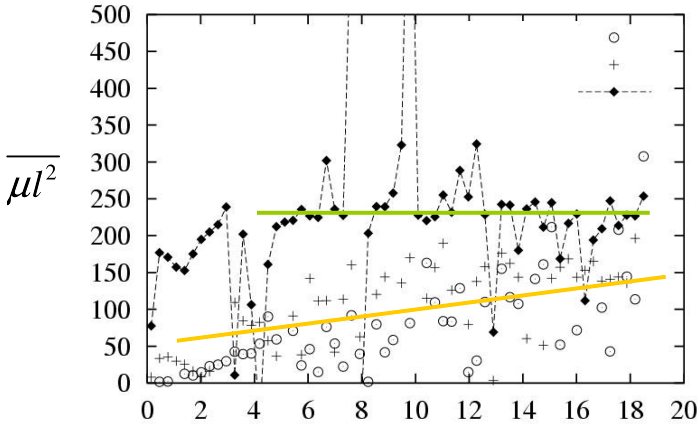
Rotations – spin density

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



Macro (torque stiffness)

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



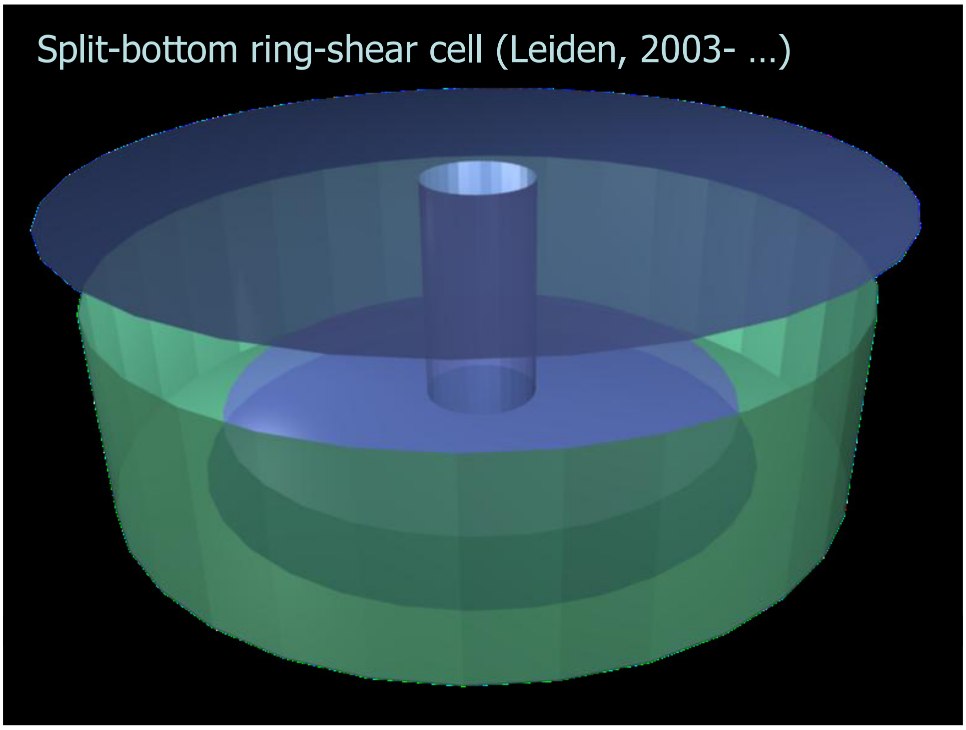
3D ring shear cell

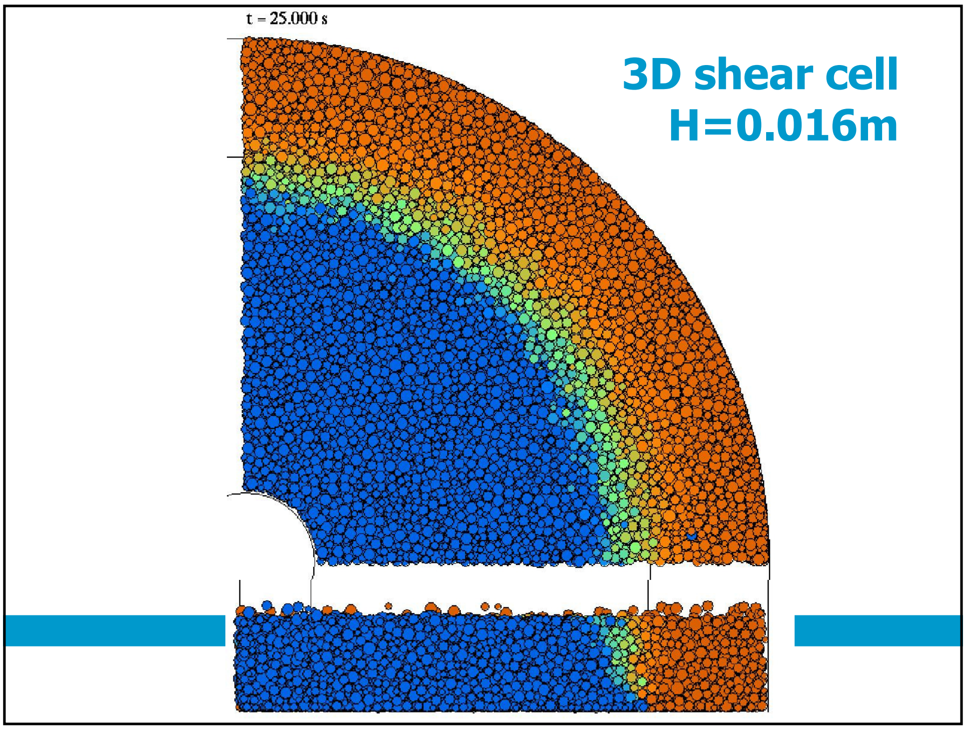
<u>local</u> micro-macro for steady shear flow

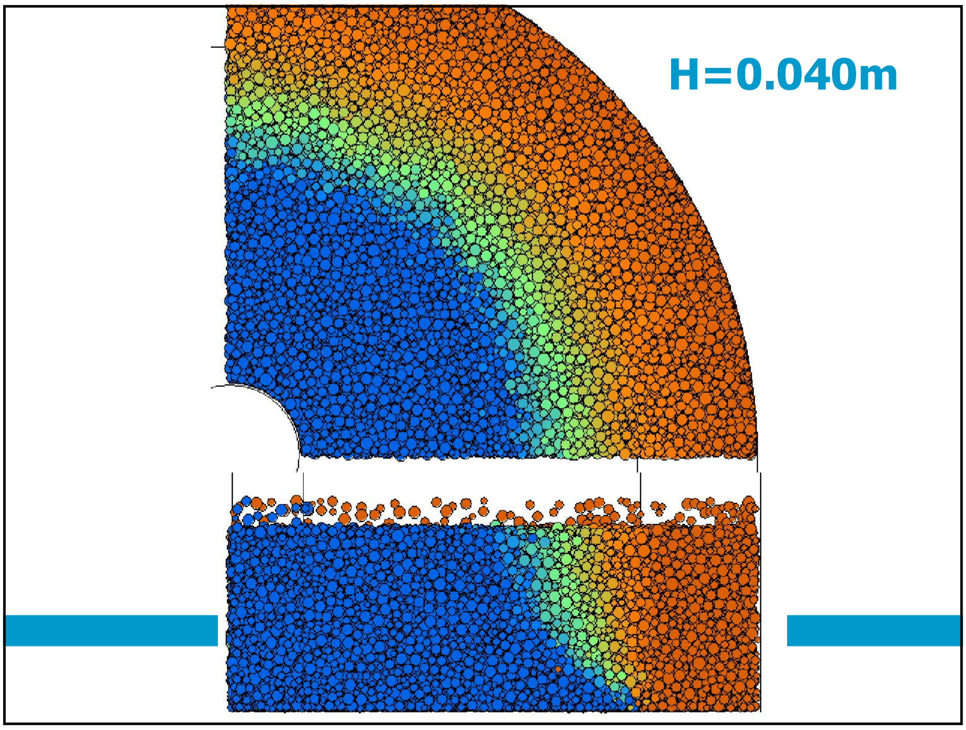
- viscosity
- yield stress
- anisotropy
- etc.

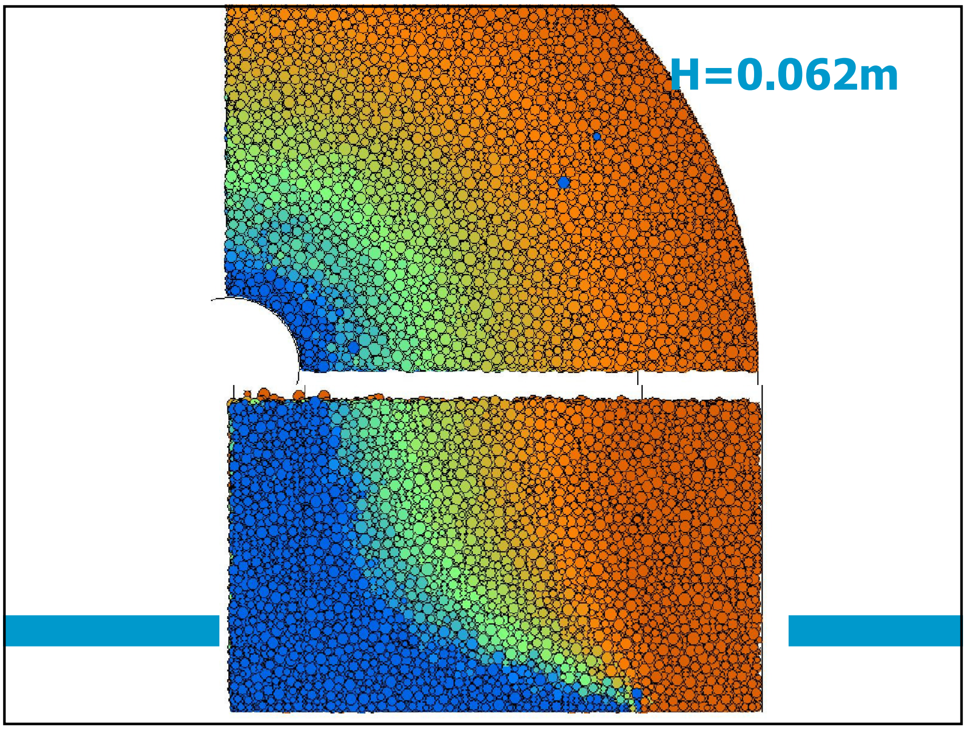
Advantages:

- shearband position known!
- long time-averaging
- space-averaging

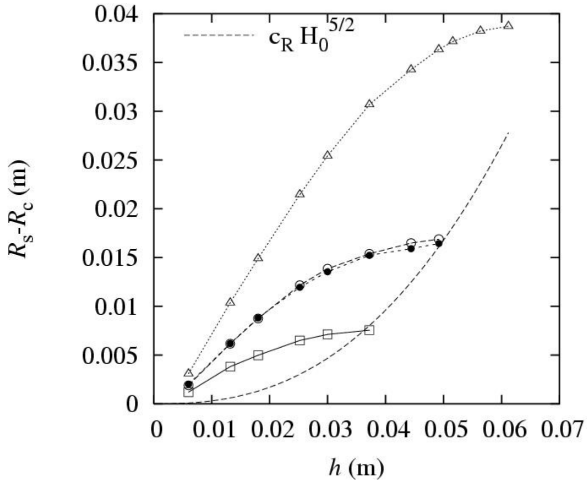

Split-bottom ring-shear cell (Leiden, 2003- …)


t = 25.000 s
3D shear cell
H=0.016m


H=0.040m

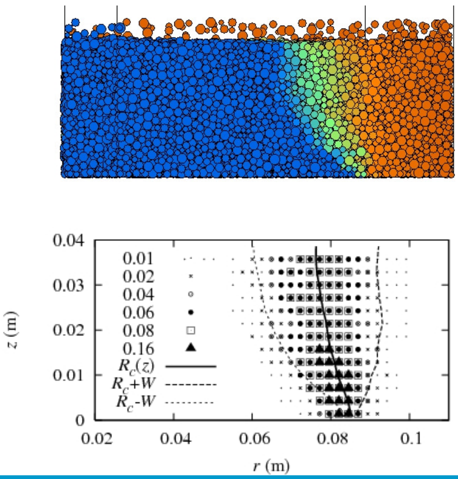

H=0.062m

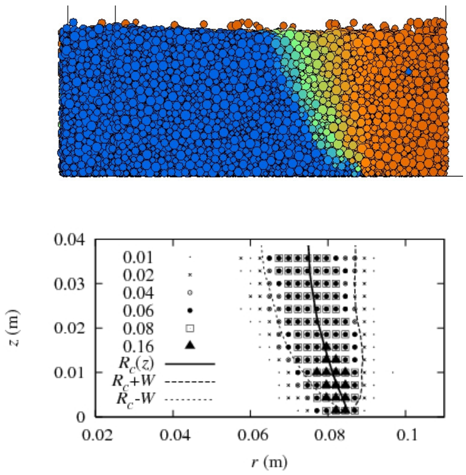
3D shear band center position



80% quantitative agreement with experiments …

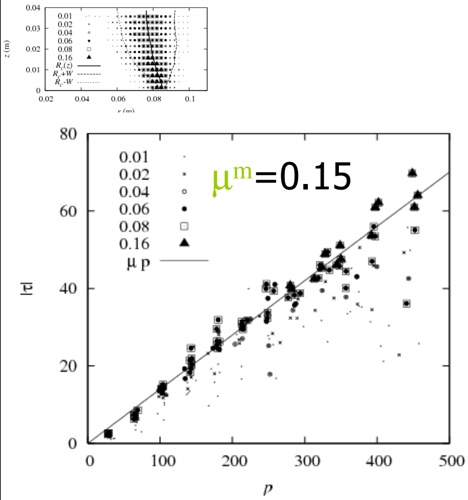
Constitutive relations – shear rate $\dot{\gamma}$

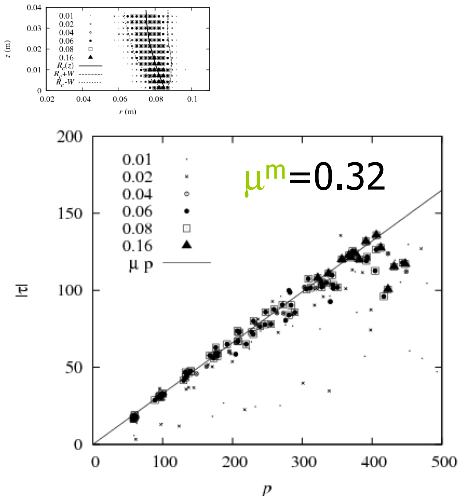




no friction friction

Constitutive relations: Mohr-Coulomb



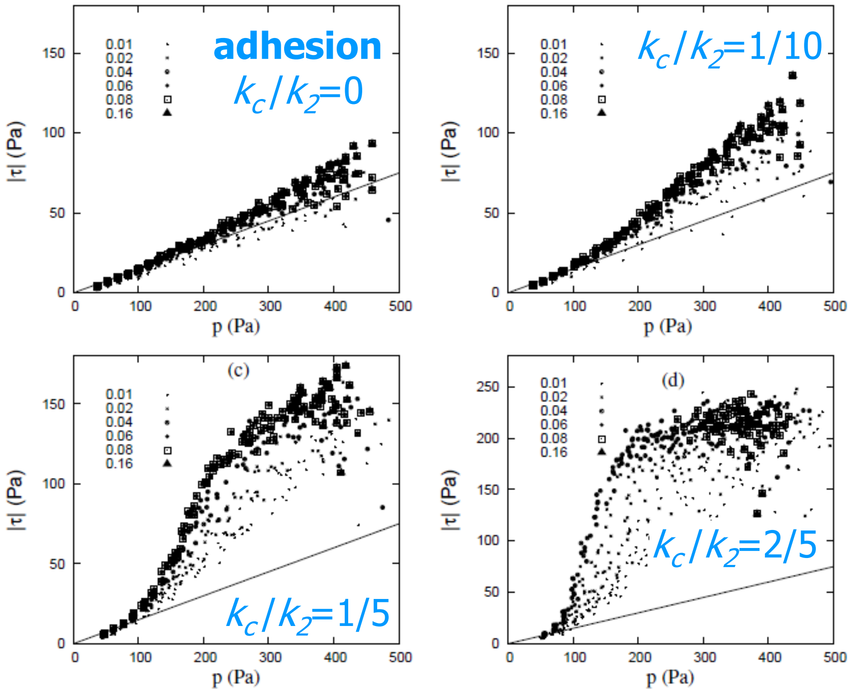


no friction μ=0 friction μ=0.4

Granular flow …

- compressibility? / dilatancy?
- **MohrCoulomb-like yield stress?**
- shear viscosity?
- inhomogeneity? (force-chains)
- (almost always) an-isotropy?
- micro-polar effects (rotations) …

NOTE: all points = 1 simulation - only

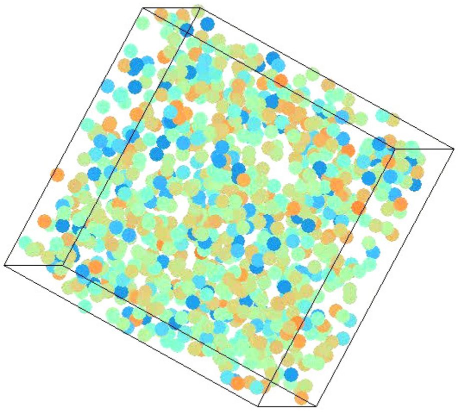


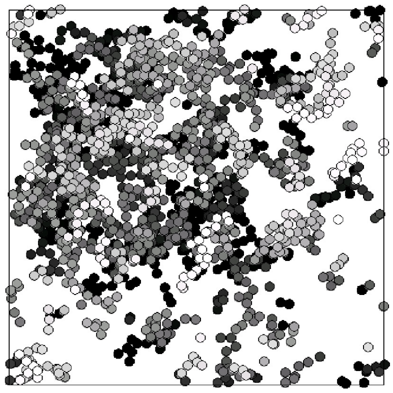
3D Flow behavior – steady state shear

Obtain LOCAL constitutive laws from one SINGLE simulation:

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

… Details of interaction





Attraction + Dissipation = Agglomeration

Summary

MD particle simulations of 3D steady shear:
+ advanced particle interaction force models
+ *micro-macro transition* (LOCAL!!!)
⇒ Yield surface … from ONE simulation
⇒ understand the interplay: micro-macro

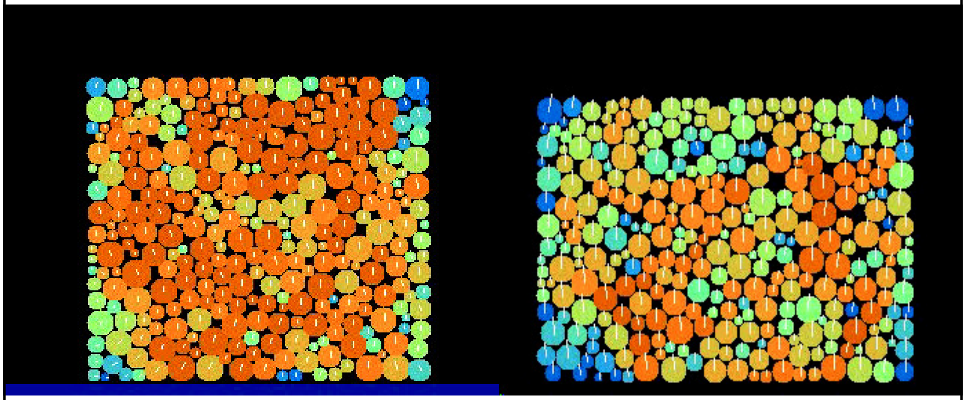
Outlook

Non-spherical particles …

Shear rate -> shear path dependence …

Sintering / Cementation

7. Vibration test

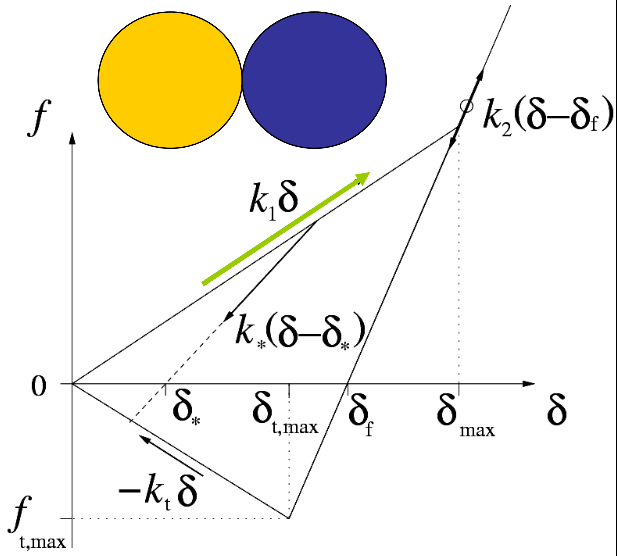


p=100 p=10

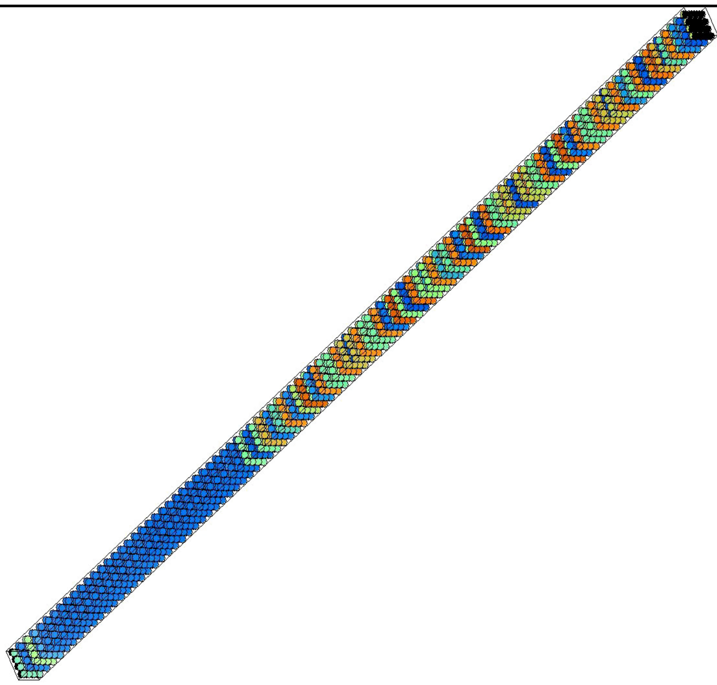
The End

Contacts

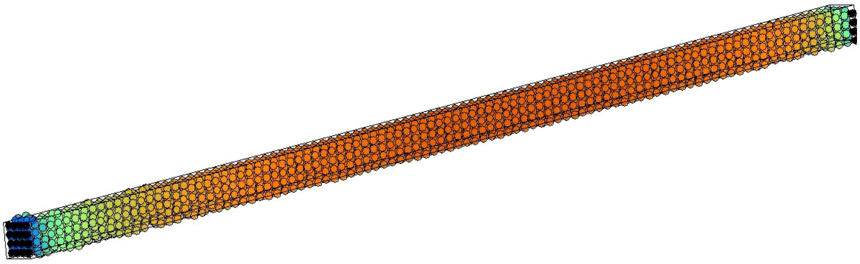
1. loading



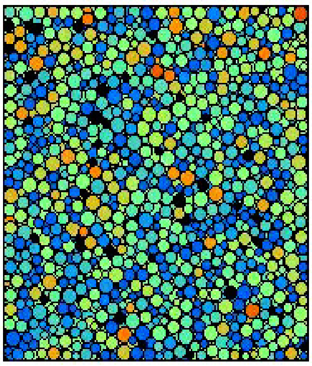
P-wave



+polydispersity $\Delta a>0$

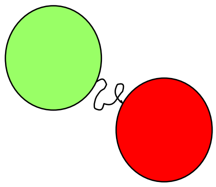


P-wave animation



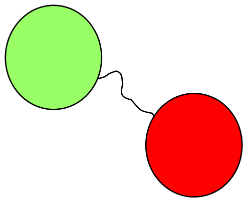
Another example: Membranes

Add strings to the hard spheres …



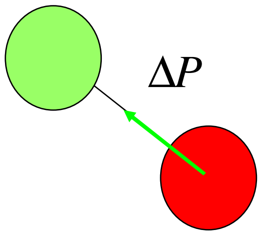
Another example: Membranes

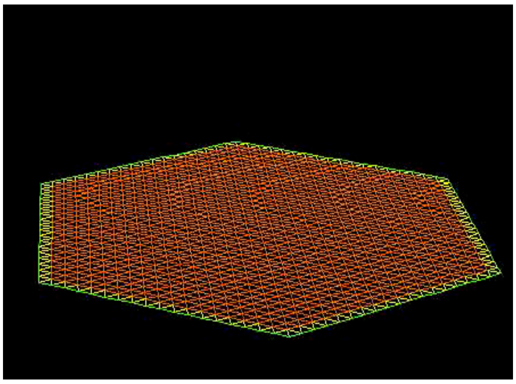
Add strings to the hard spheres …



Another example: Membranes

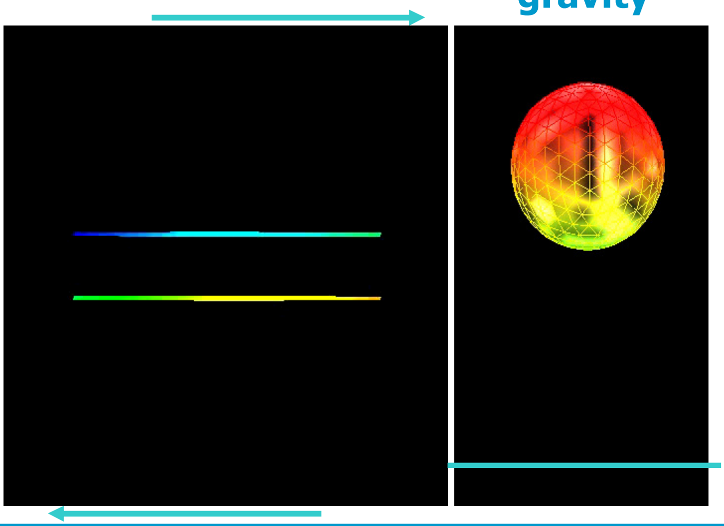
Add strings to the hard spheres …



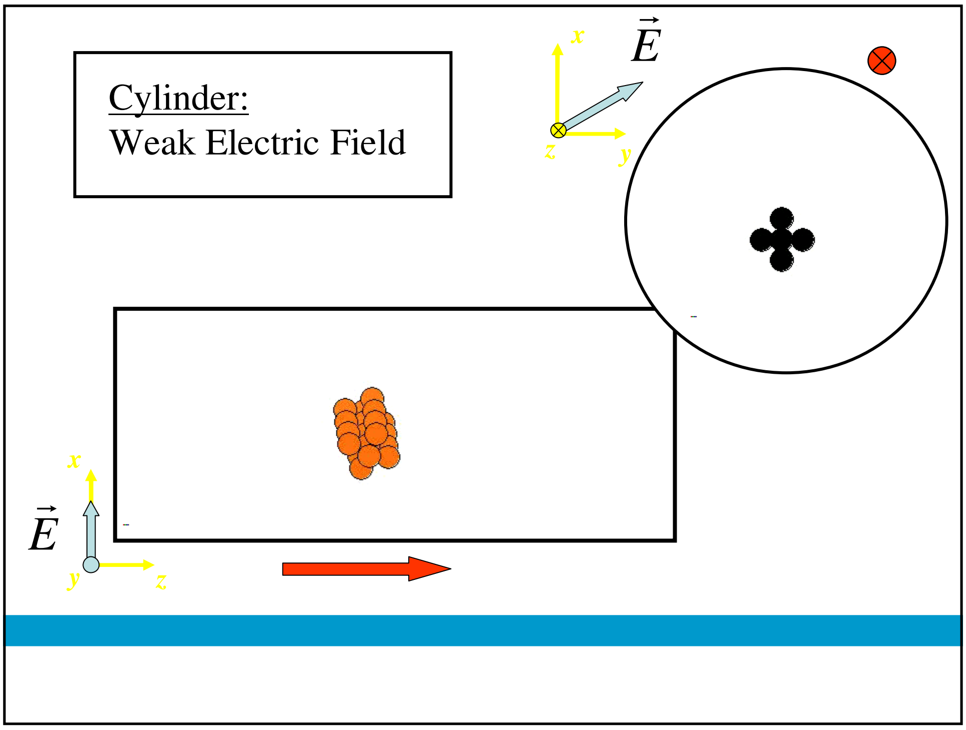


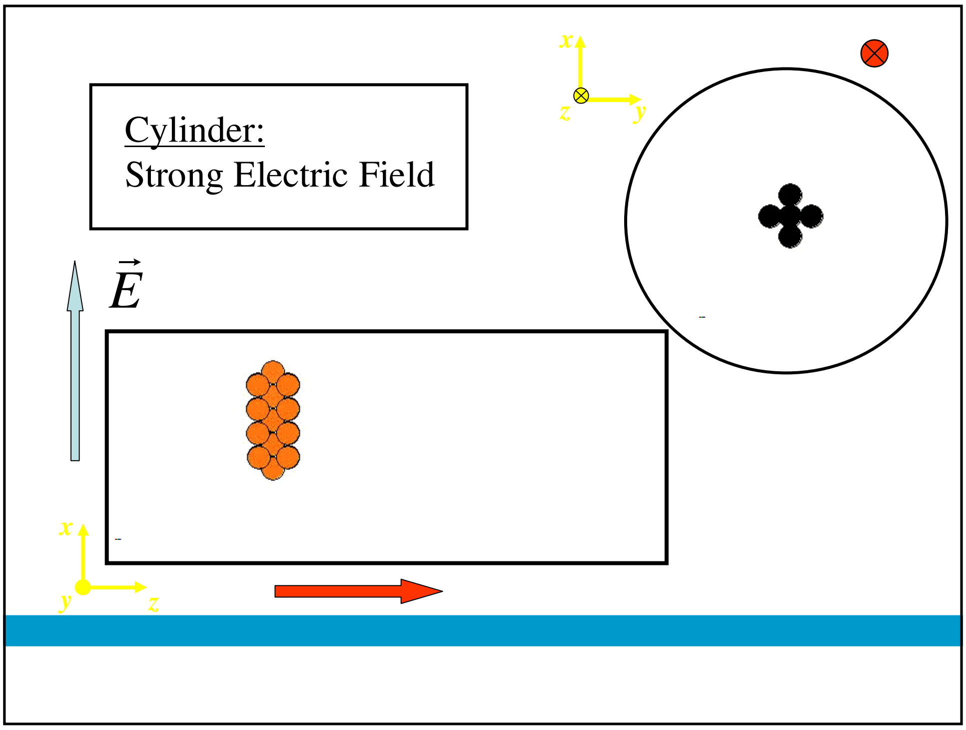
Membranes

gravity

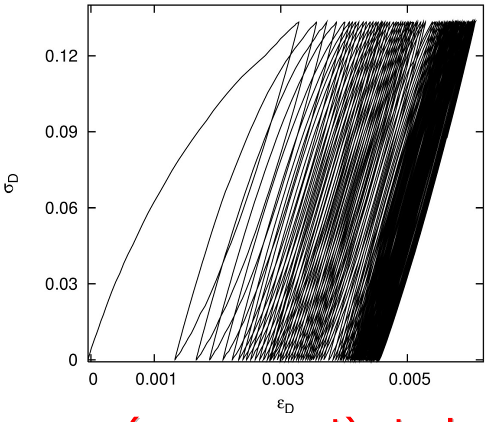


shear
-flow

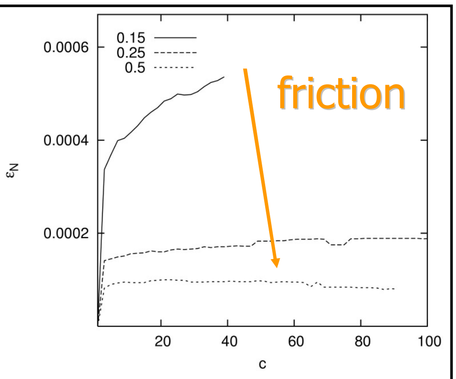

Cylinder:
Weak Electric Field
x
E
z
y
x
E
y
z

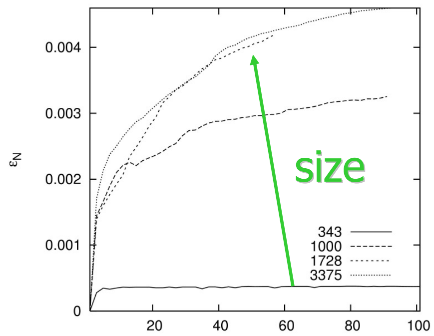

Cylinder:
Strong Electric Field
x
z
y
E
x
y
z

Ratcheting
(cyclic stress)

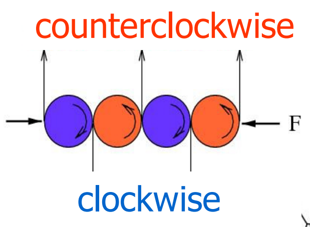


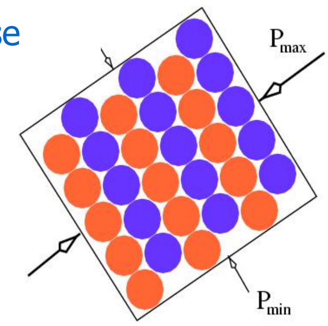
→ (permanent) strain

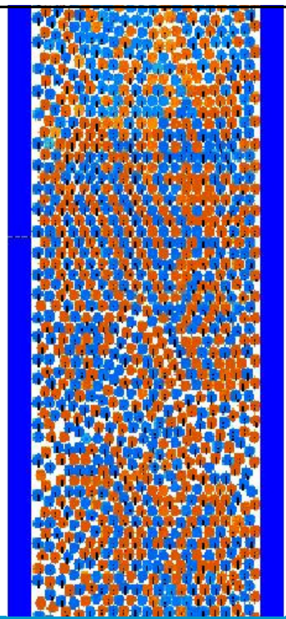




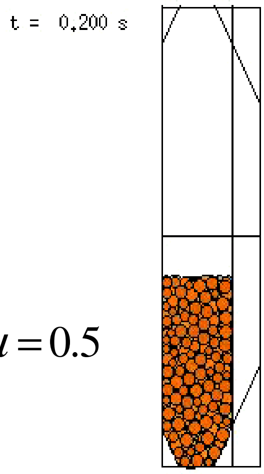
Rotational order



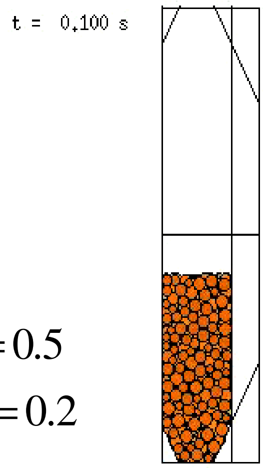




Silo Flow with friction



$\mu = 0.5$

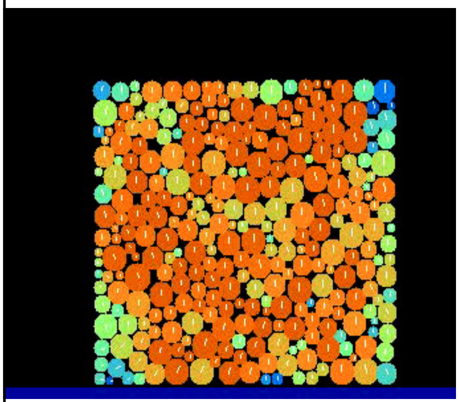


$\mu = 0.5$

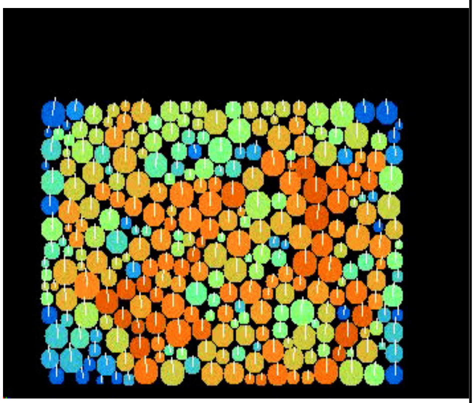
$\mu_r = 0.2$

Sintering / Cementation

7. Vibration test

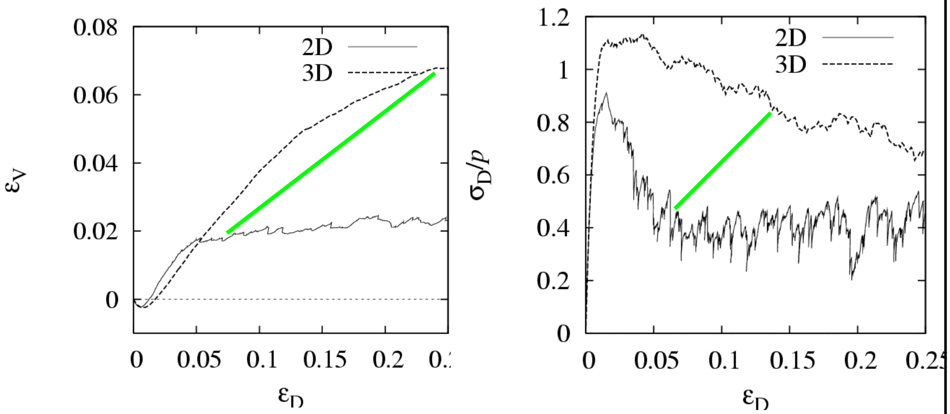


p=100



p=10

2D-3D – comparison?



- Saturation at large friction coefficients?