Particles, micro-macro, continuum theory: shear bands, memory of jamming & dilatancy

Stefan Luding, MSM, CTW, UTwente, NL

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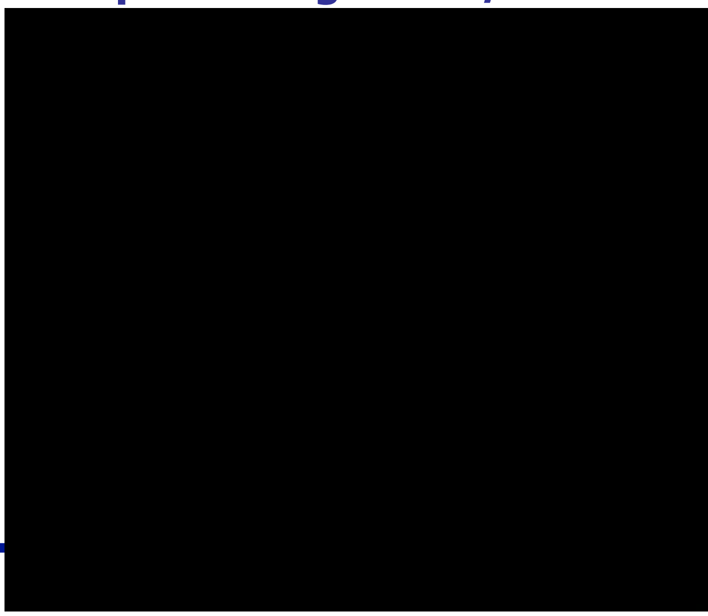
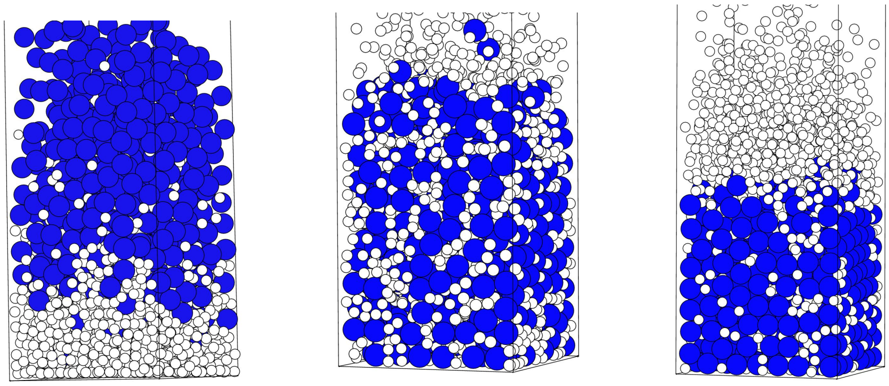
Example 1: Agitation/Vibration



LFO
next talk

N. Rivas, MSM
2011-13

Example 2: Segregation/Mixing

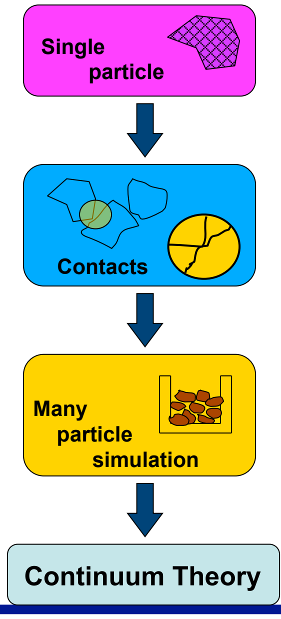


… previous talk Nico Gray

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

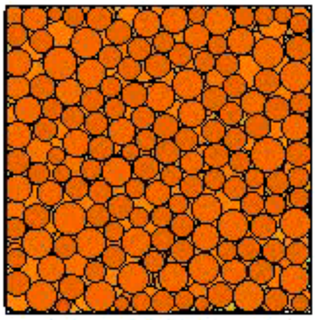
Overview

- Introduction
- Contact models
- Many particle simulation
- Global/local coarse graining
- Continuum Theory
- … Anisotropy+Dilatancy
- … **Time-scales**+Memory



Tabletting -> tension-test

$k_t / k_2 = 1/2$



Continuum theory

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

momentum conservation:

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

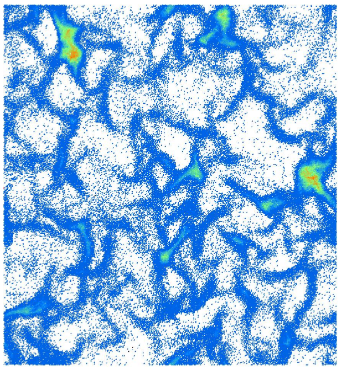
energy balance:

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

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

How to understand clustering ?

Goldhirsch, Zanetti 1993, …



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

… why ?

dissipation = energy loss (irreversible)

Freely cooling system

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

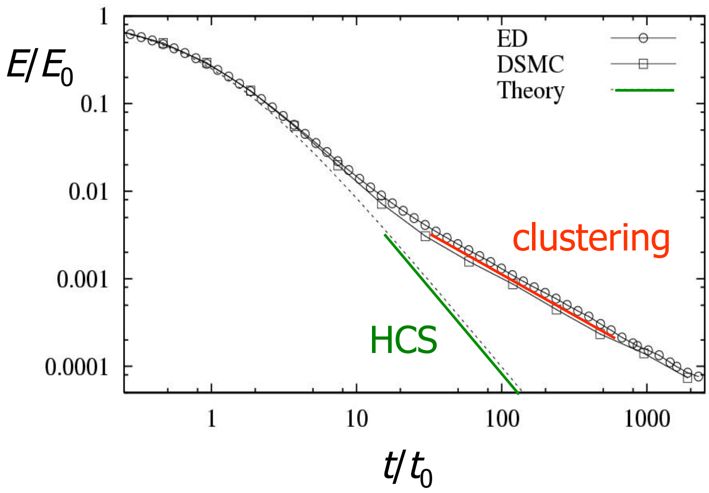
mass & momentum conservation – OK

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

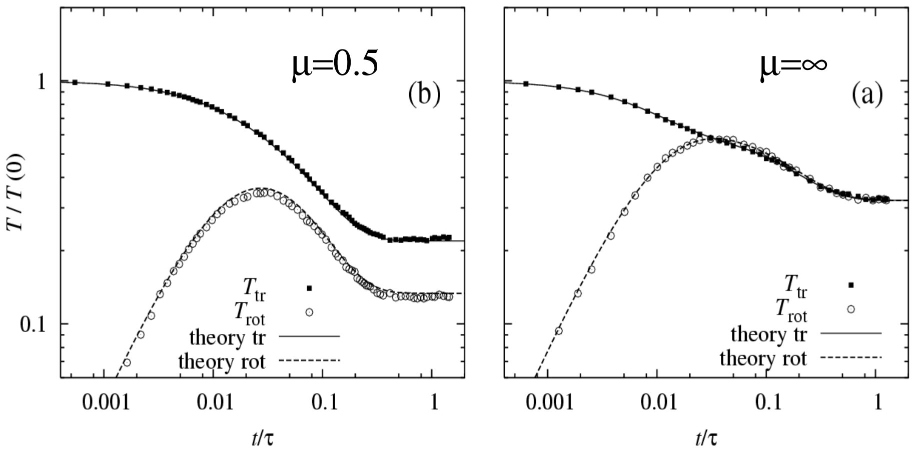
mean field (MF) solution: $$\frac{v}{v_0} = \frac{1}{1+\alpha\left(1-r^2\right)v_0 t}$$

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

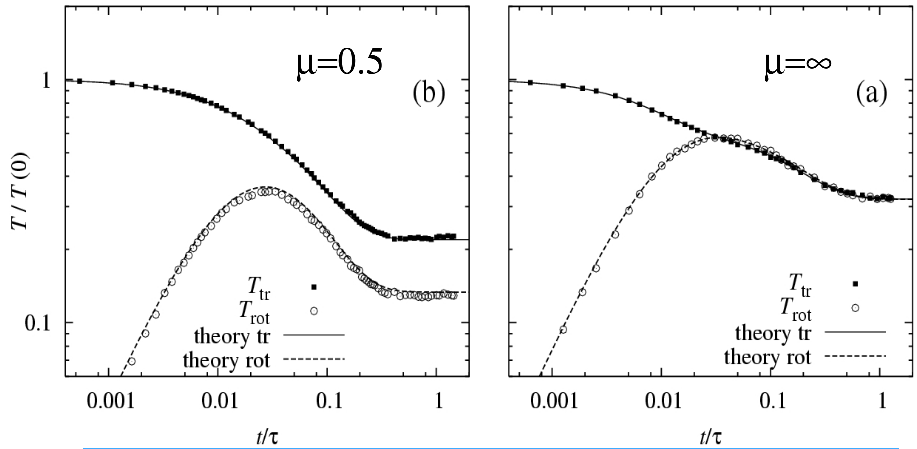
Freely cooling system (HCS)



Kinetic theory with Coulomb friction



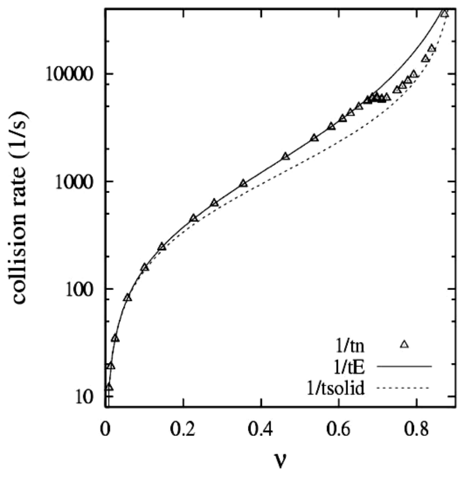
Kinetic theory with Coulomb friction



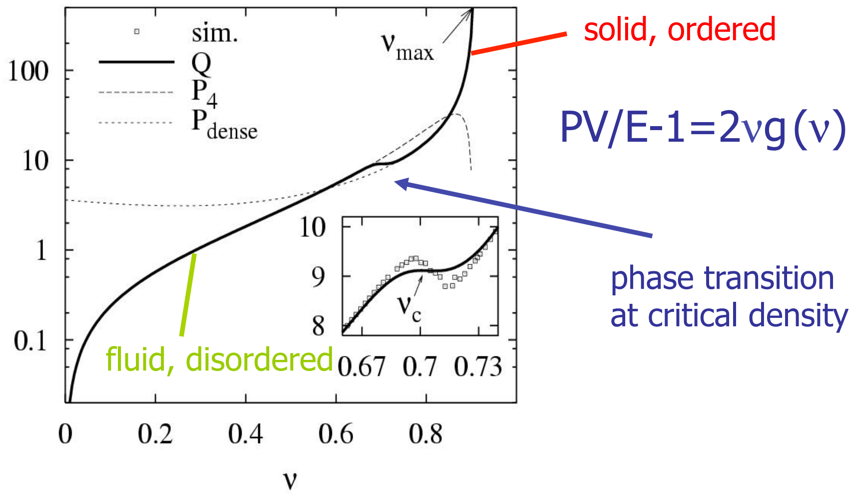
... possible, but serious hard work ...

NO shortcut

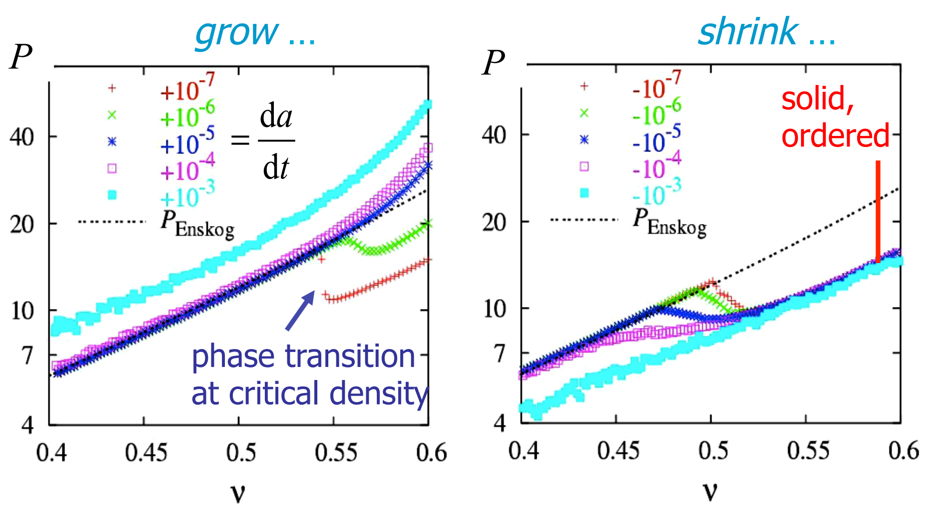
Collision rate – time scale



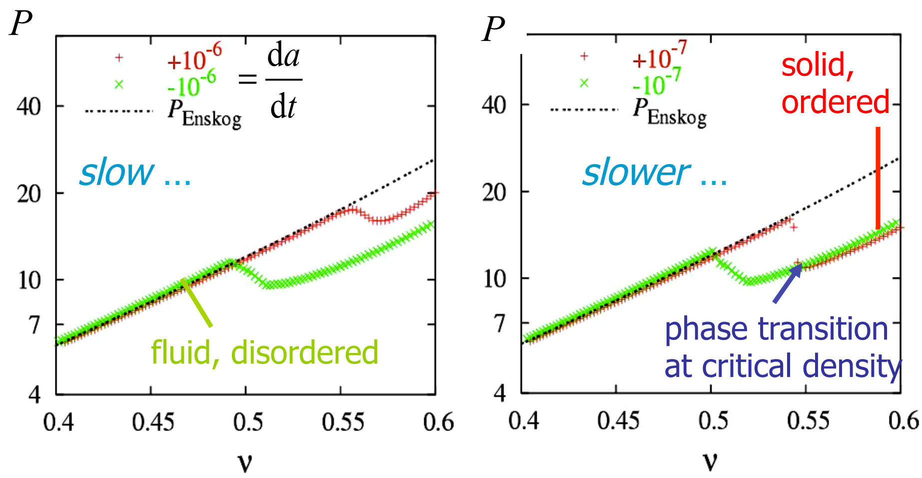
Pressure (Equation of State – 2D)



Pressure (Equation of State – 3D)



Pressure (Equation of State – 3D)



… dissipation rate

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

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:

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

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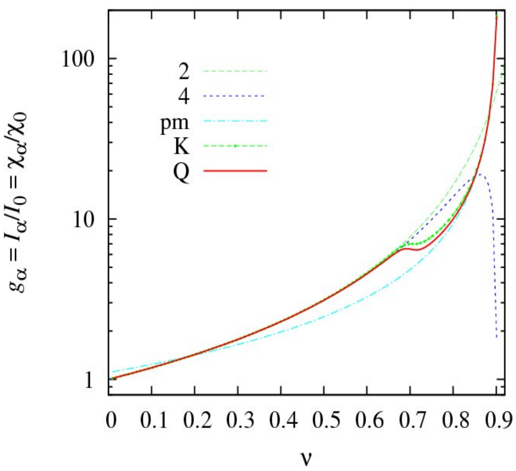
… dissipation rate



… heat-conductivity

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

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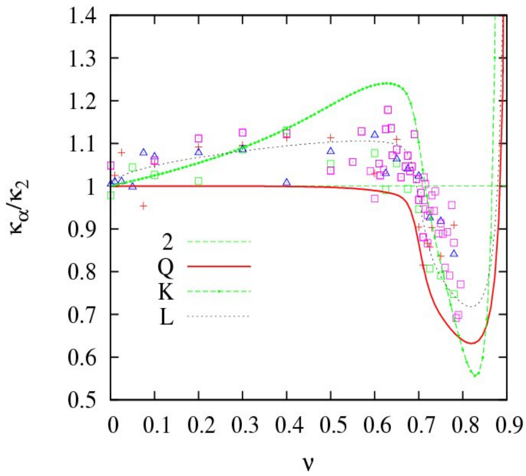
… heat-conductivity



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… shear-viscosity

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

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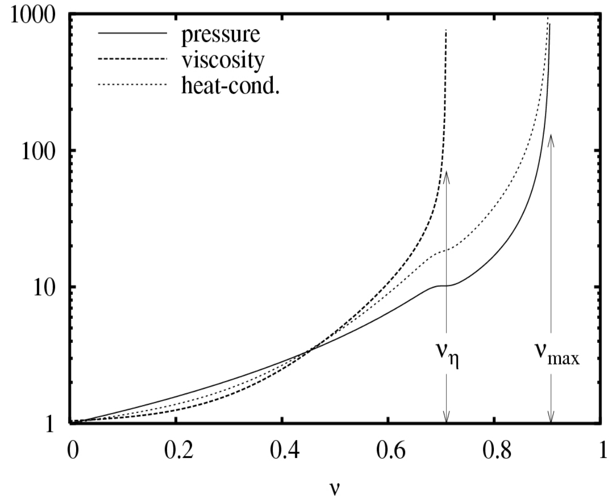
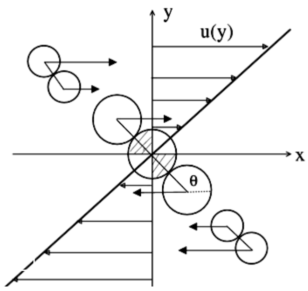
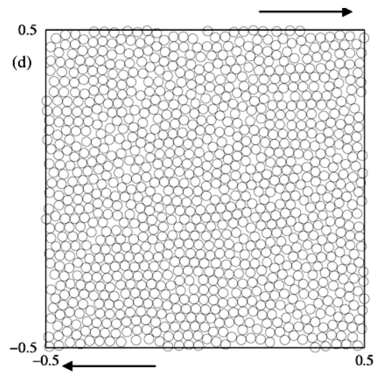
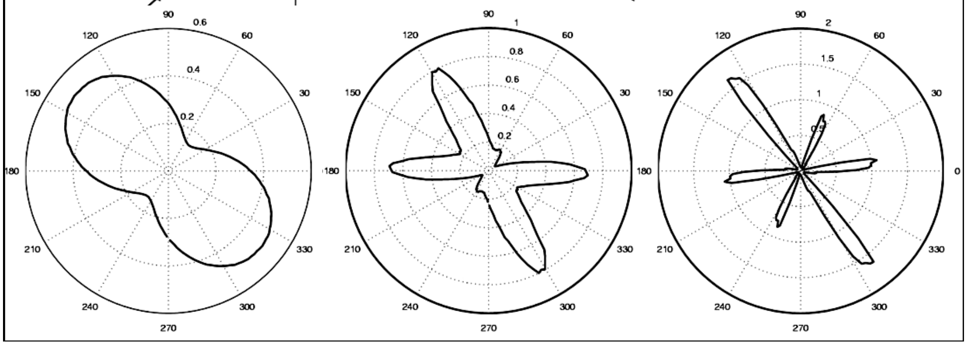
Global equations of state (2D)



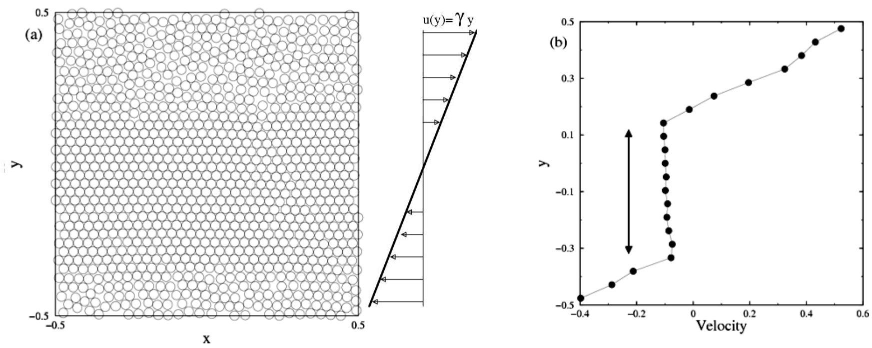
Structure formation







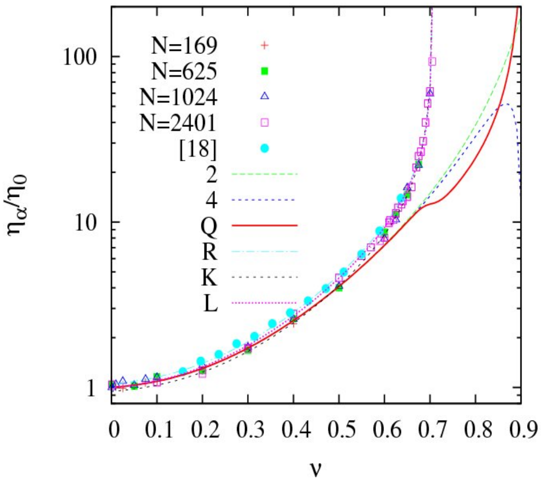
Structure formation



Low density -> linear velocity profile

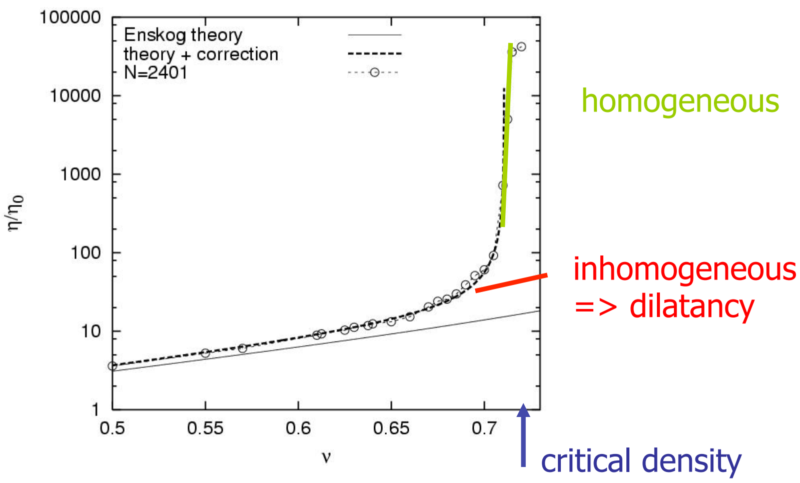
High density -> shear localization

shear "viscosity" (2D)

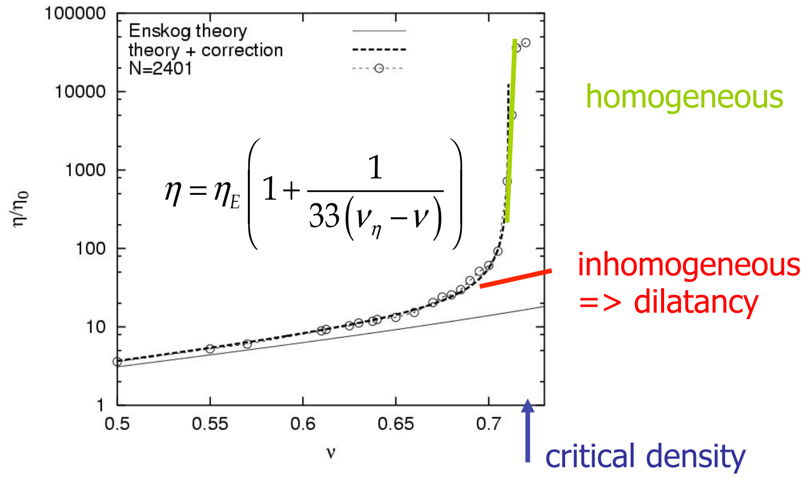


S. Luding, *Nonlinearity*, Dec. 2009

Shear (viscosity at high density)

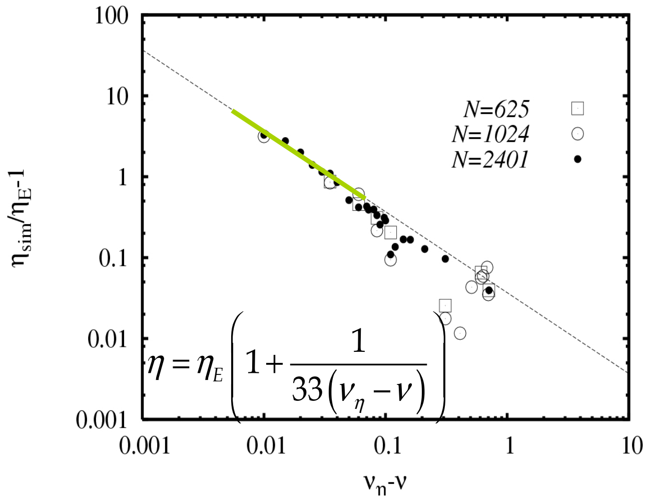


Shear (viscosity at high density)



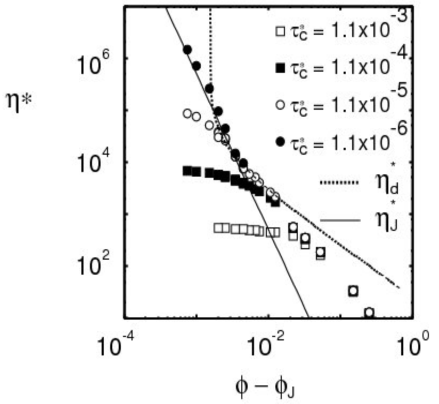
R. Garcia-Rojo, S. Luding, J. J. Brey, PRE 2006

Shear viscosity divergence: power -1



Approach to jamming

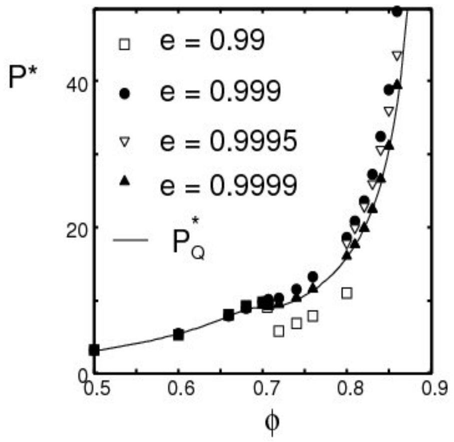
Which power law is it? … really -1?

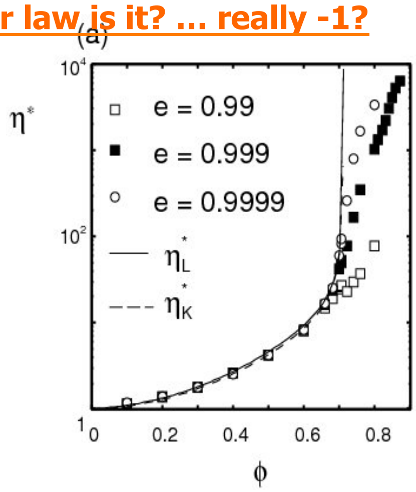


Otsuki, Hayakawa -> -3 !!!

Approach to jamming

- Which power law is it? … really -1?

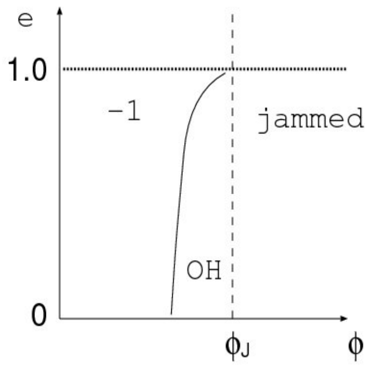


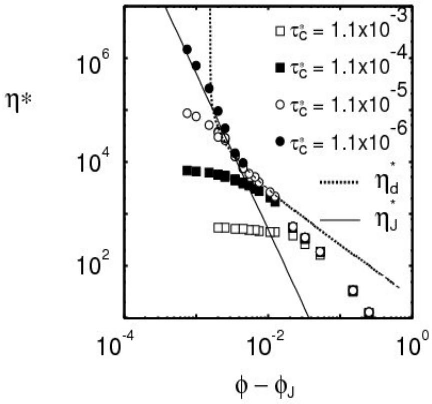


- control parameter -> dim.less. dissip.rate

Approach to jamming

- **Which power law is it? … really -1?**



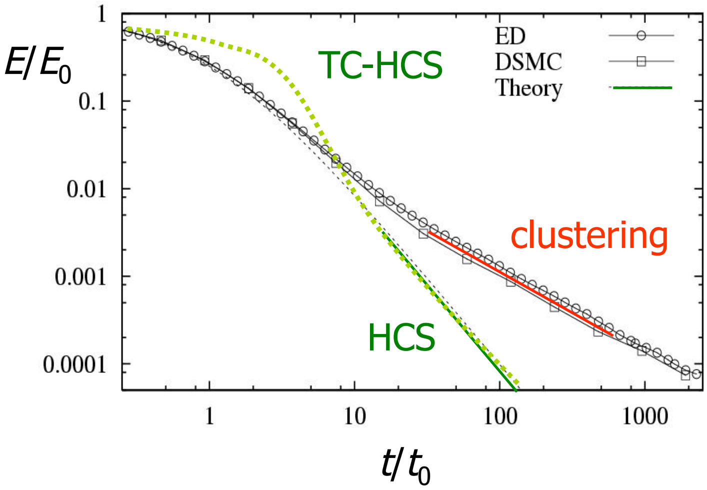


M. Otsuki, H. Hayakawa, S. Luding, JTP, 2010

Time-scales

- Time between collisions, tn
- Inverse compression/shear rate
- Contact duration tc (softness)
- Inverse dissipation rate
- (gravity = 0, up to now)
- (pressure ~ tn)

Freely cooling system (HCS->TC-HCS)

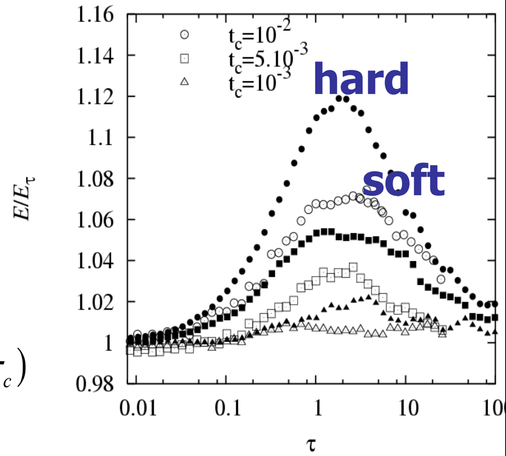


Multi-particle contacts (hard & soft!)

- Higher density, T
- multiple static contacts
- smaller dissipation

$$\tau_c = \frac{t_c}{t_n}$$

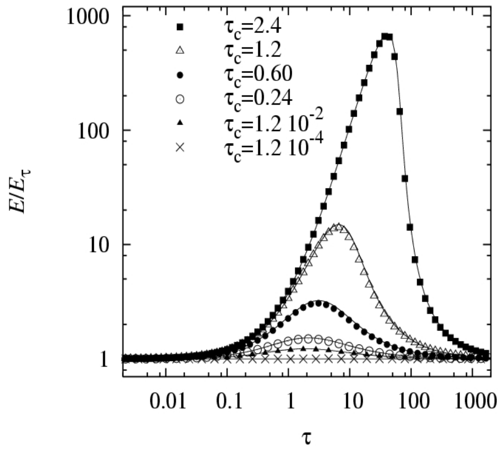
$$I \rightarrow I \exp\left(-c\frac{t_c}{t_n}\right) = I \exp(-c\tau_c)$$



Kinetic theory for multi-particle contacts

- Higher density
- Multiple, static contac
- Smaller dissipation

$$I \to I \exp(-\alpha \tau_c)$$



Static vs. dynamic
another order parameter?

TC model allows to define

- "potential" energy
- "static" contacts

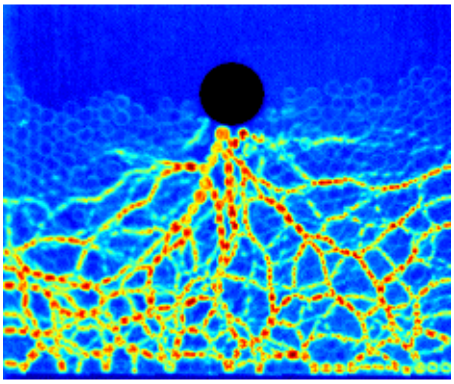
$$\tau_c := \frac{t_c}{t_n} > 1: \quad \text{static}$$

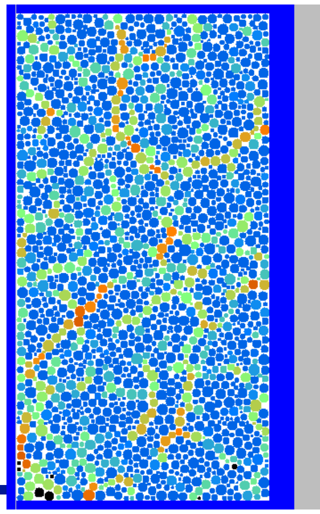
$$\tau_c := \frac{t_c}{t_n} < 1: \quad \text{collisional}$$

$$+\text{dynamic}$$

go beyond the limits of
hard sphere model validity …

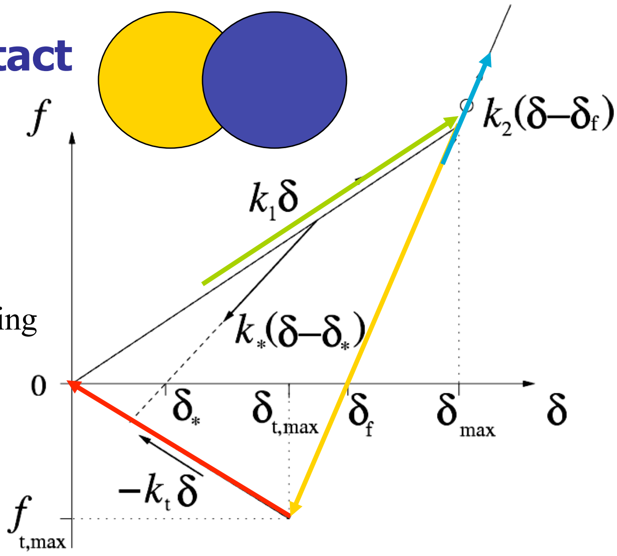
Force-chains
experiments - simulations



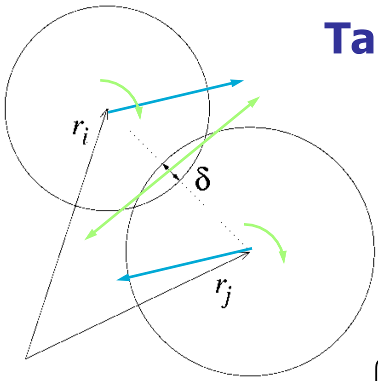


Cohesive contact

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

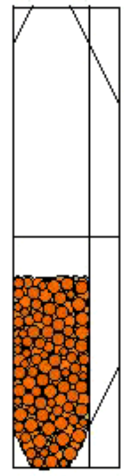


Sliding **contact points:**
- **static Coulomb friction**
- **dynamic Coulomb friction**
- **objectivity**

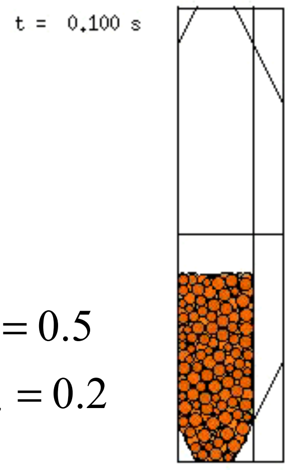
Sliding/Rolling/Torsion

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

Flow with friction & rolling resistance



$\mu = 0.5$



$\mu = 0.5$

$\mu_r = 0.2$

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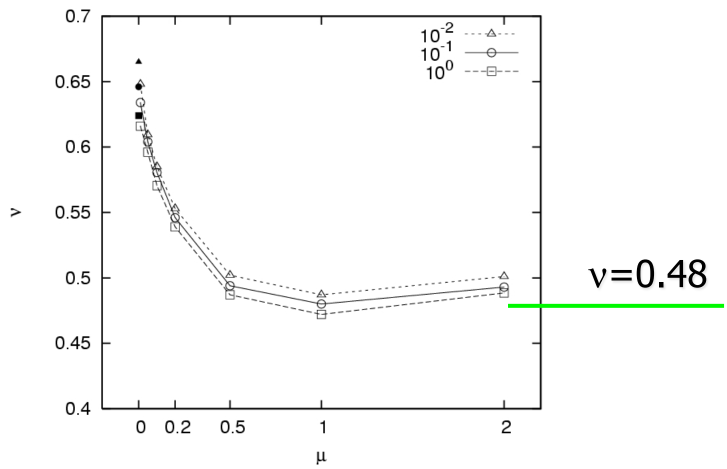
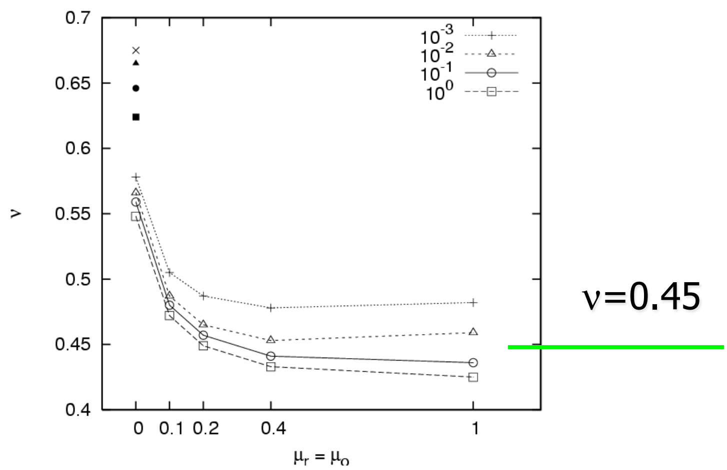
3D – Density vs. friction …



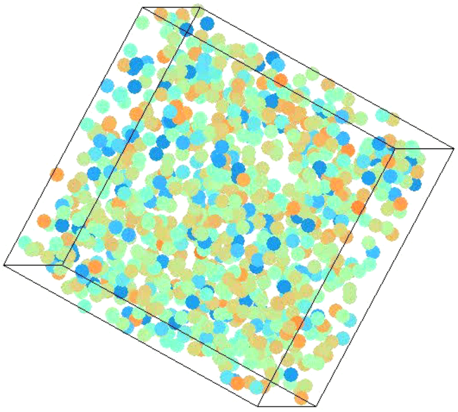
- Saturation at strong friction

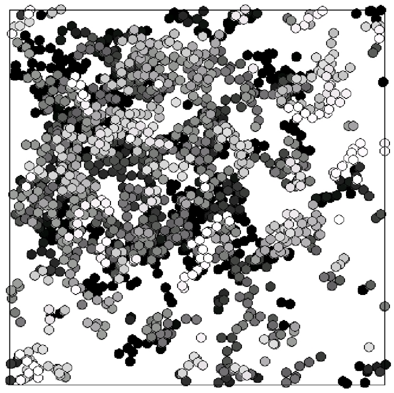
3D – Density vs. rolling-resistance



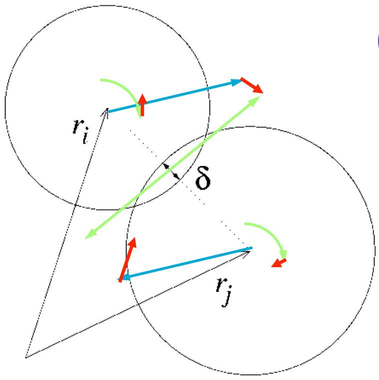
- Saturation at high rolling resistance

… details of interaction





Attraction + Dissipation = Agglomeration

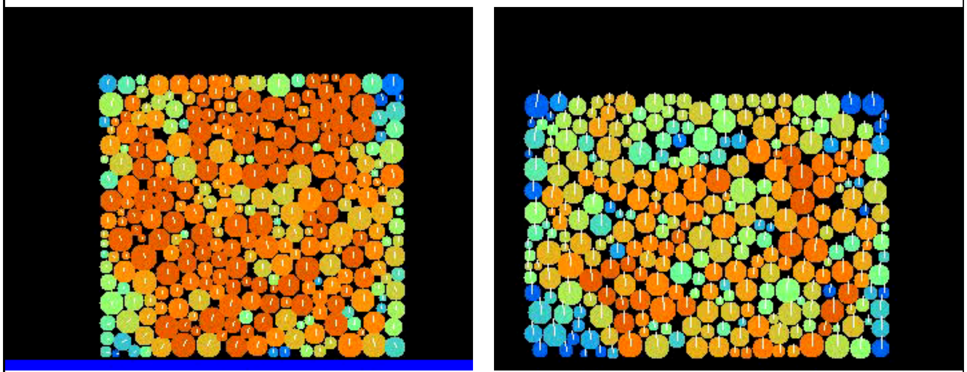


(Random) Fluctuations

- *thermostat?*
- Brownian dynamics
- …
- Hydrodynamics
- …
- electric fields
- temperature
- …

Sintering – Temperature dependence

Vibration test



p=100 p=10

Biaxial box element test

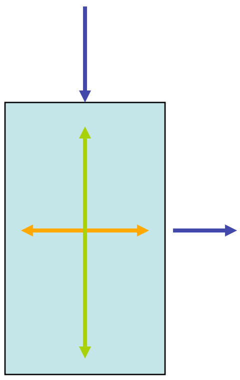
- Top wall: strain controlled

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

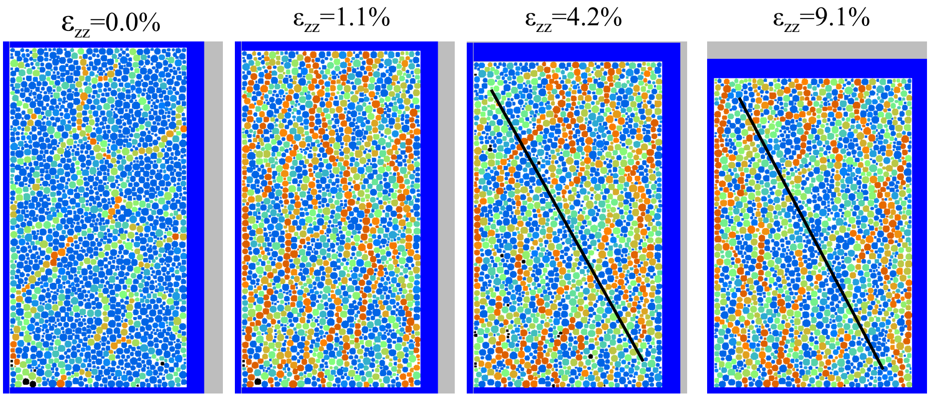
- Right wall: stress controlled

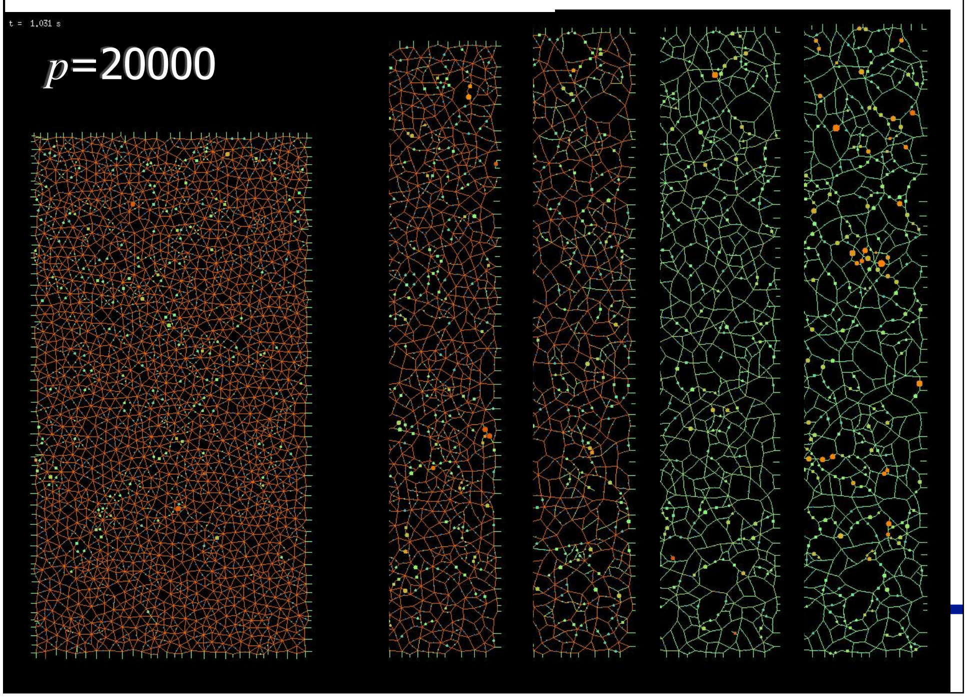
$$p = \text{const.}$$

- Evolution with time … ?

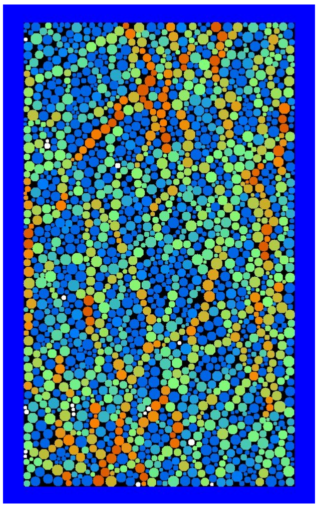


Element test simulations





Bi-axial box (stress chains)



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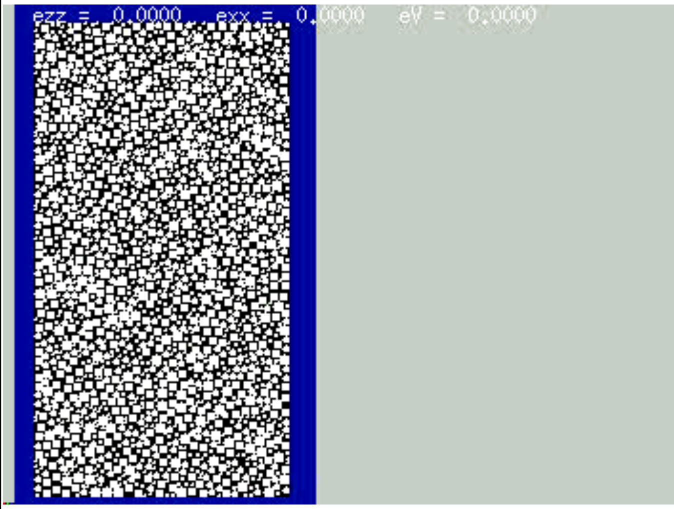
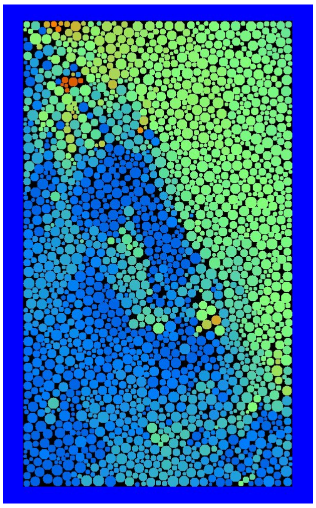
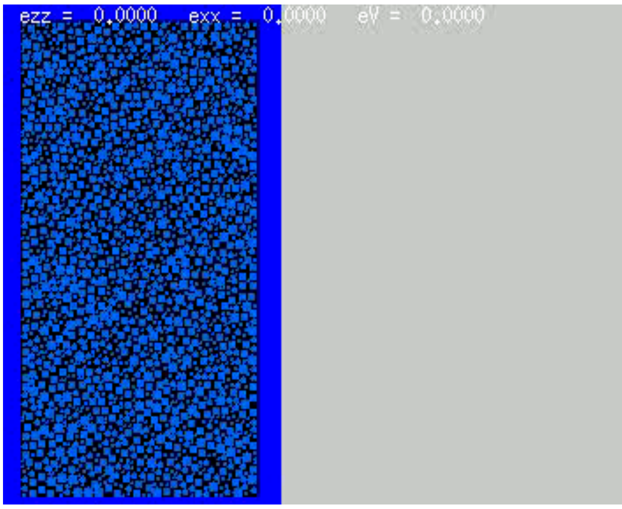


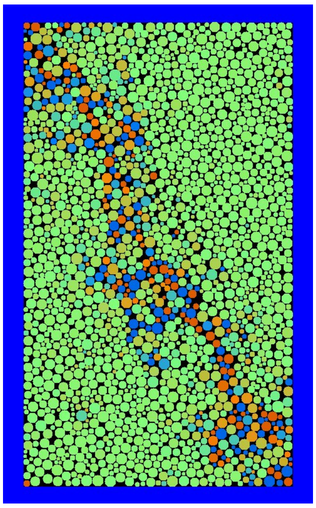
Bi-axial box (kinetic energy)



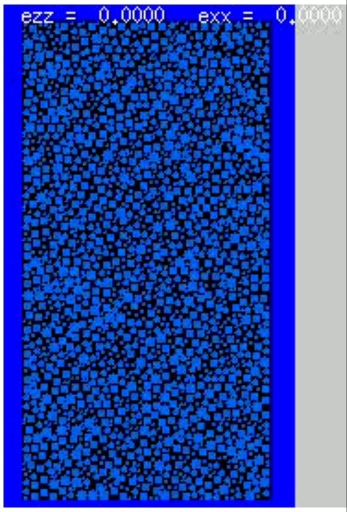
Bi-axial box (kinetic energy)



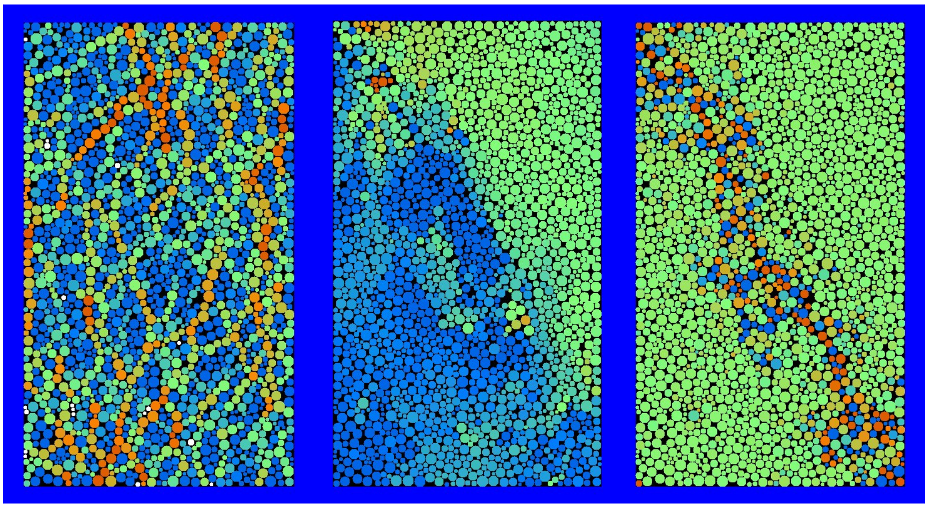
Bi-axial box (rotations)



Bi-axial box (rotations)

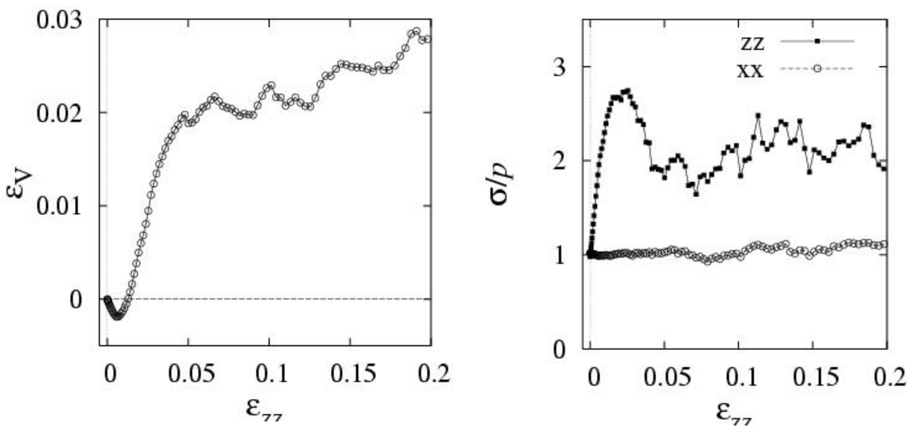


Multiple micro-mechanisms

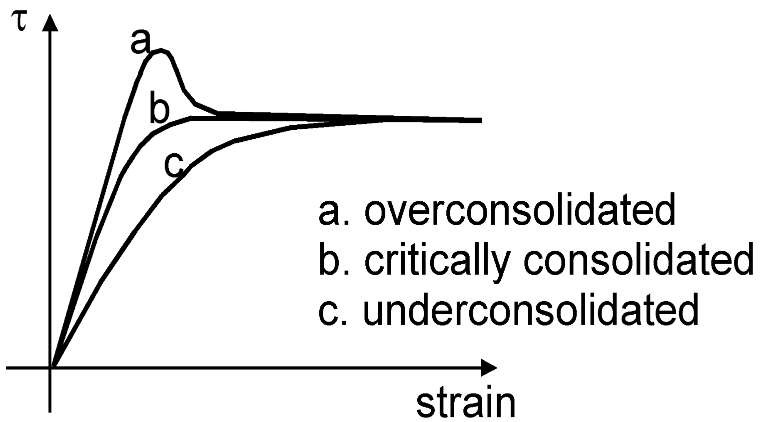


inhomogeneity & anisotropy, instabilities & structures, rotations

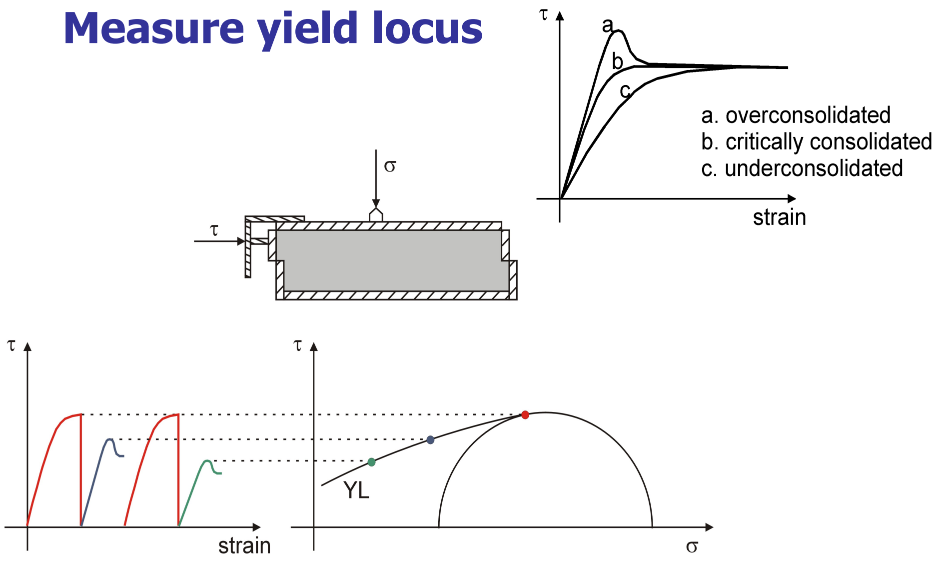
Bi-axial compression with p_x=const.



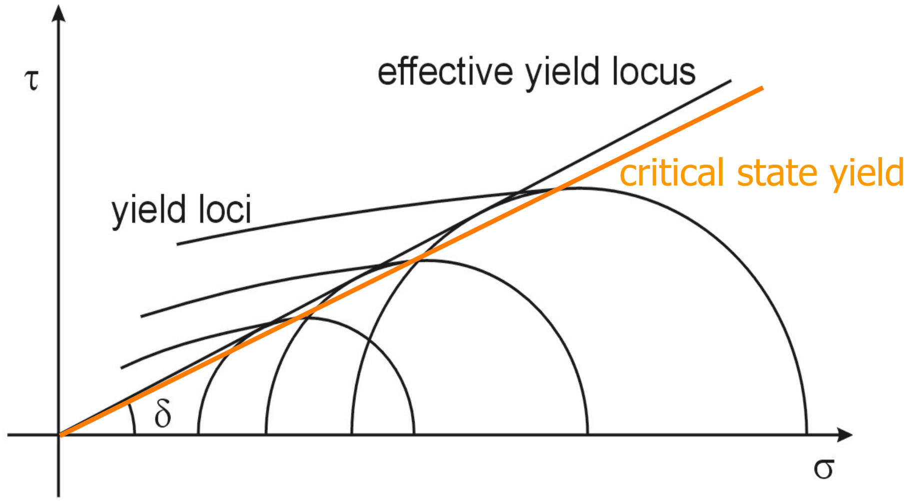
Microscopic interpretation: memory?



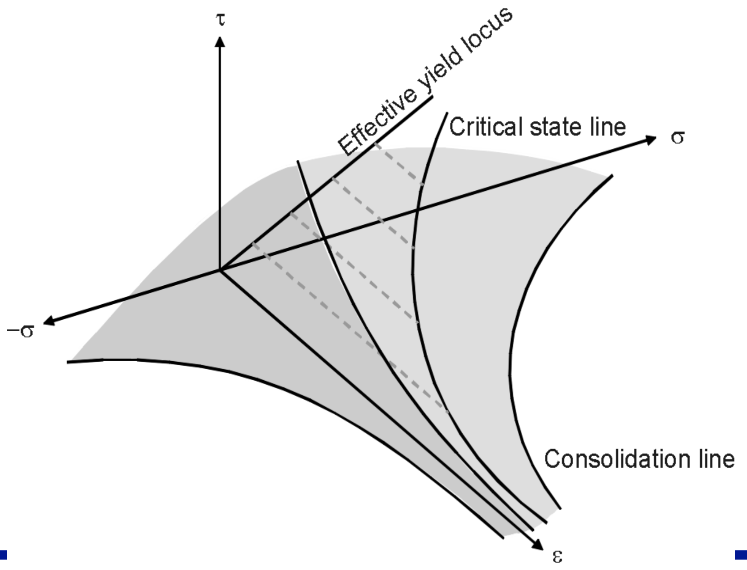
Measure yield locus



Yield loci

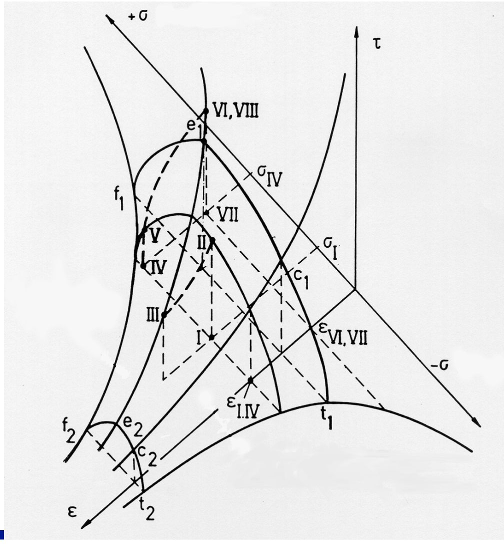


Hvorslev diagram (-50 years) <-> jamming diagram

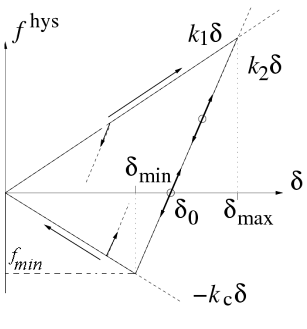


porosity = 1 - volume fraction

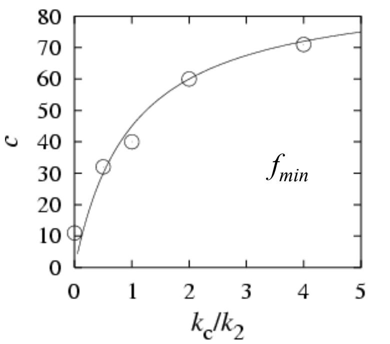
Consolidation and Failure Surfaces



Micro-macro for cohesion

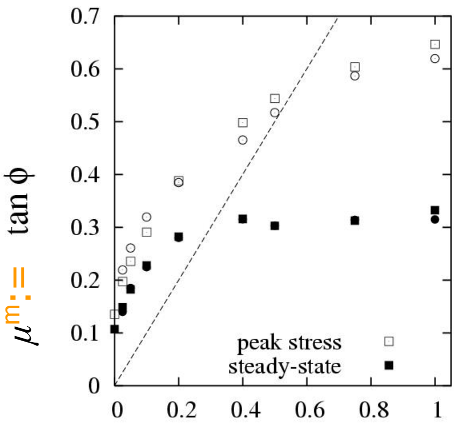


$k_c / k_2 = 0, 1/2, 1, 2, \text{and } 4$



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

Micro-macro for friction



prepared μ=0

prepared μ=0.5

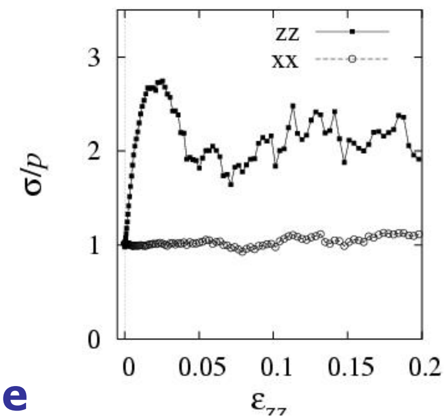
steady-state shear

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

NOTE: each point = 5-10 simulations

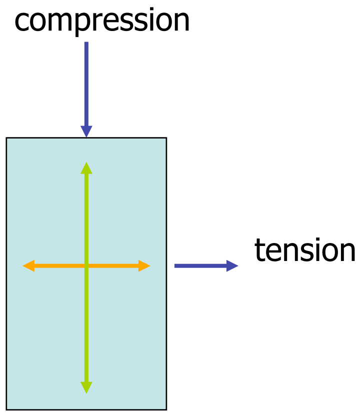
What is relevant?

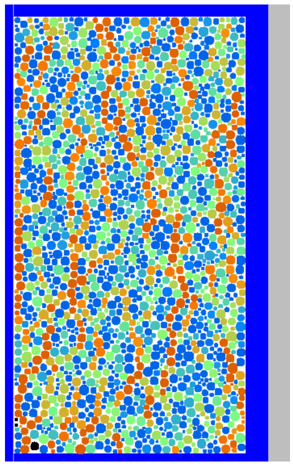
1 – critical state
2 – anisotropy …



How to find a simple constitutive model?

Micro-macro for anisotropy – rheology



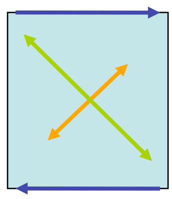


Anisotropy ⬄ Shear ?

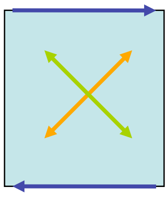
- Simple shear

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

Rotation + symmetric shear



Anisotropy ⇔ Shear ?



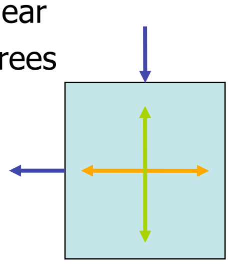
- Simple shear

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

Rotation + symmetric shear

- Rotate symmetric shear tensor by 45 degrees

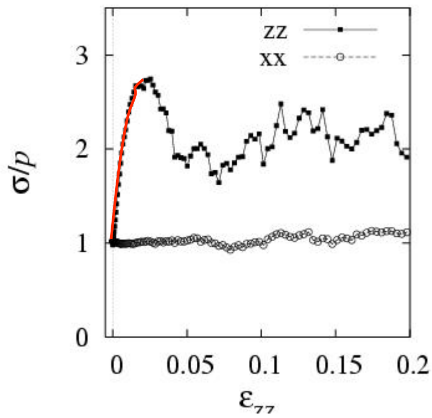
$$R_{45} \cdot \begin{pmatrix} 0 & \varepsilon_s \\ \varepsilon_s & 0 \end{pmatrix} \cdot R_{45}^T = \begin{pmatrix} \varepsilon_s & 0 \\ 0 & -\varepsilon_s \end{pmatrix}$$



- Biaxial “shear”: compression+extension

An-isotropy

in stress



An-isotropy (Stress)

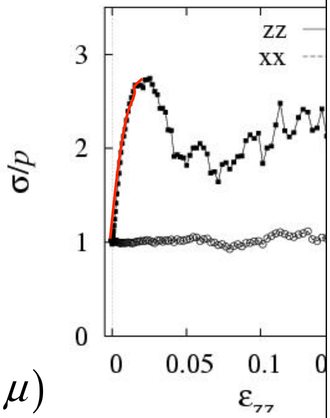
- Stress: Isotropic: tr σ, and deviatoric: dev $\sigma = \sigma_{zz}$-σ_{xx}
  - Minimal eigenvalue: σ_{xx}
  - Maximal eigenvalue: σ_{zz}
- Dev. Stress fraction $s_D = \text{dev}\,\sigma / \text{tr}\,\sigma$

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

- Exponential approach to peak

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

$$\beta_s \left(\rho, p, \mu \right)$$

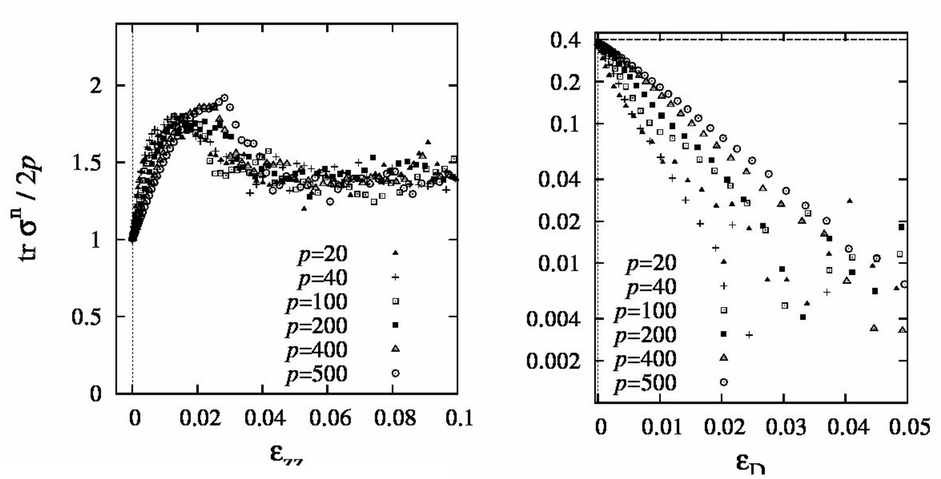


An-isotropy (Stress)

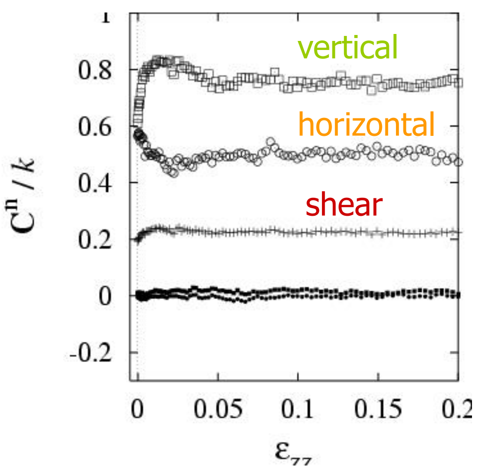
$$\frac{\partial}{\partial \varepsilon_D} s_D = \beta_s \left(s_{\max} - s_D \right)$$

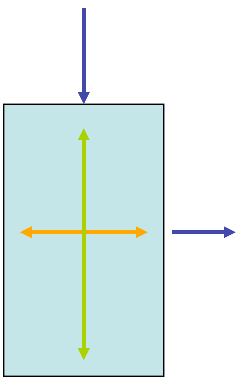
Stress (homog.)

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



Stiffness tensor





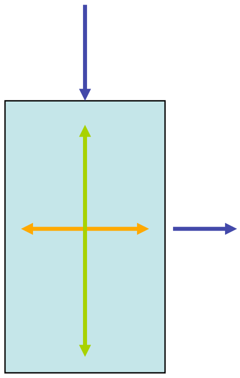
Different moduli:

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

An-isotropy (Structure)

- Structure changes with deformation
- Different stiffness:
  - More stiffness against shear C_2
  - Less stiffness perpendicular C_1
- One (only?) shear modulus
- Anisotropy $A = C_2 - C_1$ evolution

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

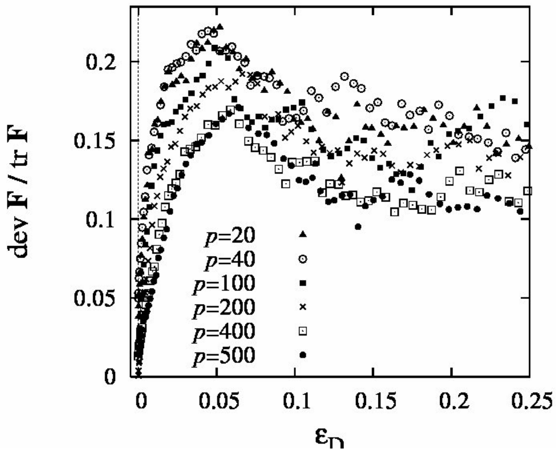


- Exponential approach to maximal anisotropy

... see Calvetti et al. 1997

Fabric

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



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)

Isotropic stress $\delta p = \delta\sigma_V = 2B\varepsilon_V + AS\,d\gamma$

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

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

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 – isotropic mat.
scalar! (in the biaxial box eigen-system)

Isotropic stress $\delta\sigma_V = 2B\varepsilon_V$

Deviatoric stress $\delta\tau = 2GS\,d\gamma$

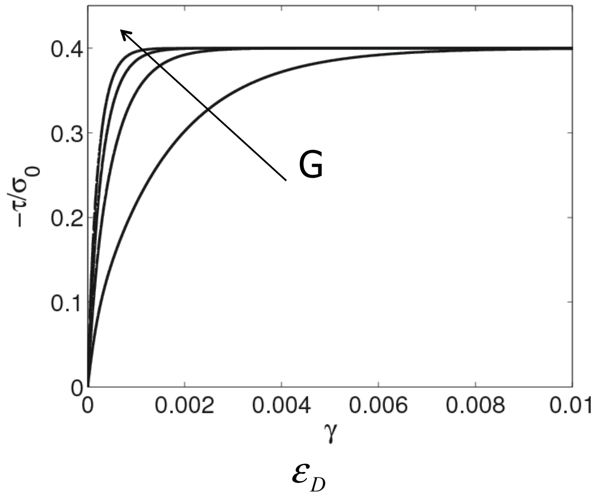
Anisotropy $A = 0$

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



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)

Constitutive model – isotropic (mode 0)

scalar! (in the biaxial box eigen-system)

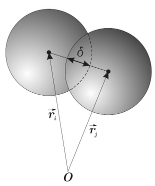
Isotropic stress	$\delta\sigma_V = 2B\varepsilon_V$
Deviatoric stress	$\delta\tau = A\varepsilon_V$
Anisotropy	$\delta A = 0$

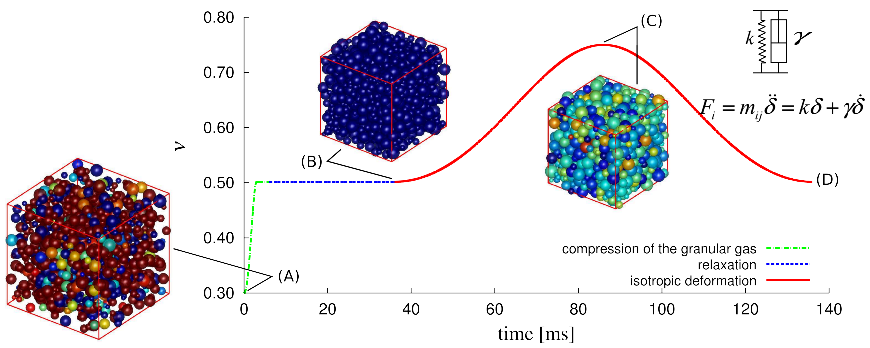
Isotropic|deviatoric strain increment $\varepsilon_V \mid d\gamma$

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

Mode 0 – Isotropic - Setup

- DEM: Frictionless polydisperse spherical particles
- Cube shape volume, periodic boundary conditions
- Linear visco-elastic contact force



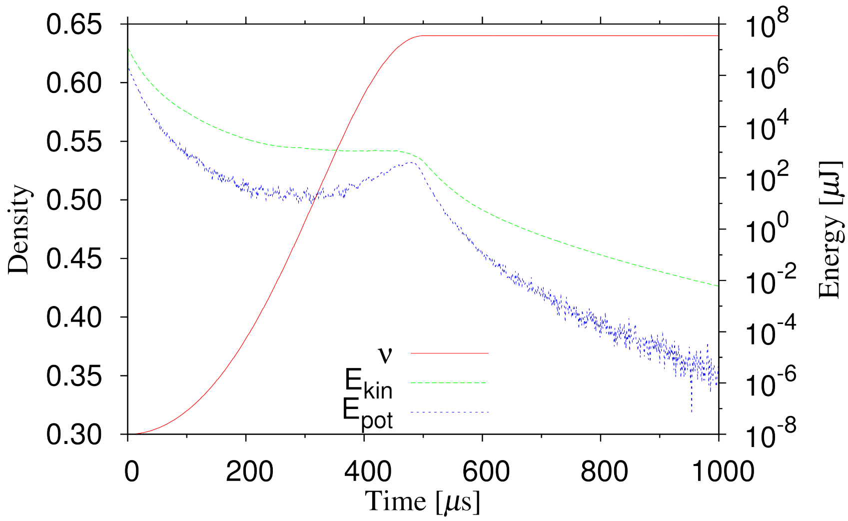


Simulation parameters

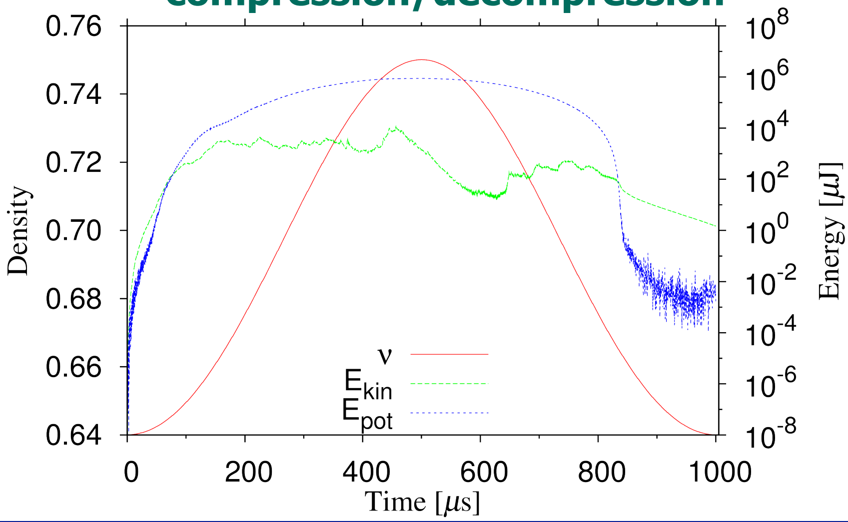
F. Goncu and S. Luding, CRAS, 2010

Parameter	Value	Description
N	1000−9261 [–]	Number of particles
$\langle r \rangle$	1 [mm]	Average radius
w	1−5 [–]	Polydispersity parameter $w = r_{\max}/r_{\min}$
ρ	2000 [kg/m^3]	Density
k_n	10^8 [kg/s^2]	Stiffness–normal spring
k_t	2×10^7 [kg/s^2]	Stiffness–tangential spring
μ	0−100 [–]	Coefficient of friction
γ_n	1 [kg/s]	Viscous dissipation–normal direction
γ_t	0.2 [kg/s]	Viscous dissipation–tangential direction
γ_{tr}	0.01 [kg/s]	Background damping–Translation
γ_{rot}	0.002 [kg/s]	Background damping–Rotation
τ_c	0.64 [μs]	Duration of a normal collision for an average size particle

Evolution of energy during preparation



Evolution of energy during compression/decompression



Coordination number

N : Total number of particles

$N_4 := N_{C\geq4}$: Number of particles with at least 4 contacts

M : Total number of contacts

$M_4 := M_{C\geq4}$: Total number of contacts of particles with at least 4 contacts

$C^r := \frac{M}{N}$: Coordination number (classical definition)

$C := C^m = \frac{M_4}{N}$: Coordination number (modified definition)

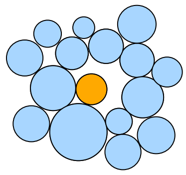
$C^* := \frac{M_4}{N_4} = \frac{C}{1-\phi_r}$: Corrected coordination number

$\phi_r := \frac{N-N_4}{N}$: (Number) fraction of rattlers

$\nu := \frac{1}{V}\sum_{p\in N} V_p$: Volume fraction of particles

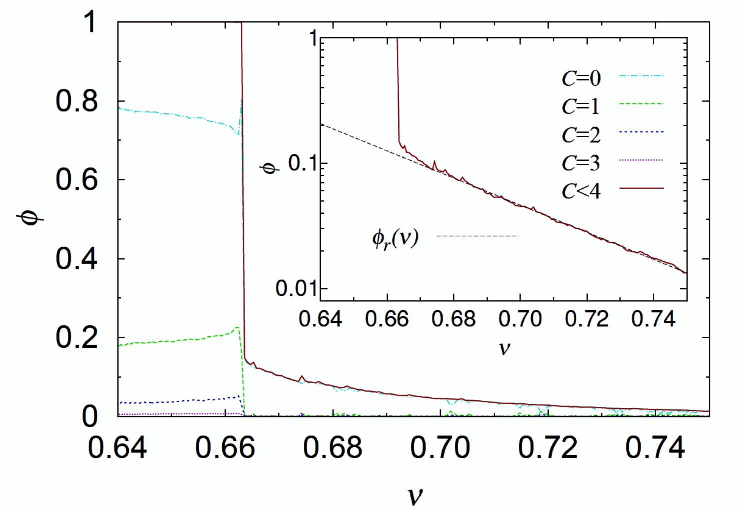
$\nu^* := \nu - \nu_r = \frac{1}{V}\sum_{p\in N_4} V_p$: Volume fraction of particles excluding rattlers

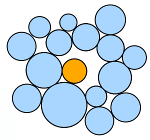
$\nu_r := \frac{1}{V}\sum_{p\notin N_4} V_p$: Volume fraction of rattlers



Coordination number – Fraction of rattlers

$$\phi_r(\nu) = \phi_c \exp\left[-\phi_\nu \left(\frac{\nu}{\nu_c} - 1\right)\right]$$



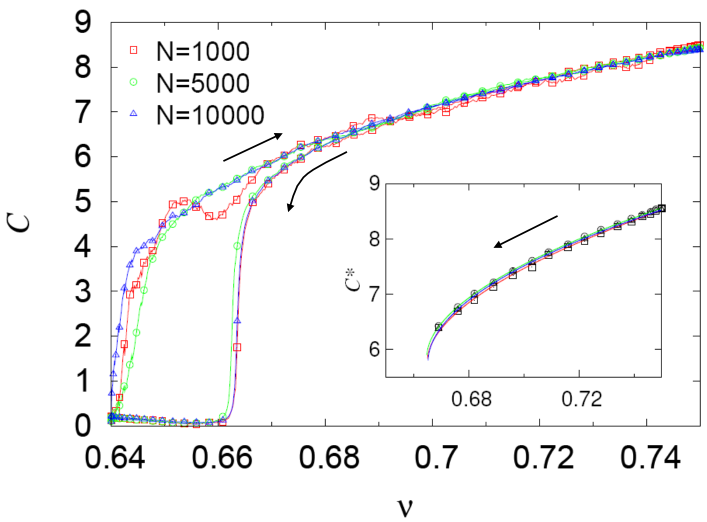


$\nu_{C*} = 0.6648$

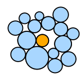
$\nu_{\phi_r} = 0.6636$

Coordination number
Effect of System size

$$C^*(\nu) = C_0 + C_1 \left(\frac{\nu}{\nu_c} - 1\right)^\alpha$$



$C<4$



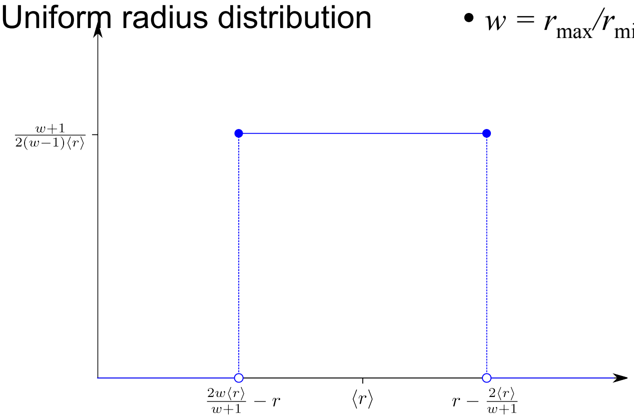
$\nu_{N=1000} = 0.6650$

$\nu_{N=5000} = 0.6647$

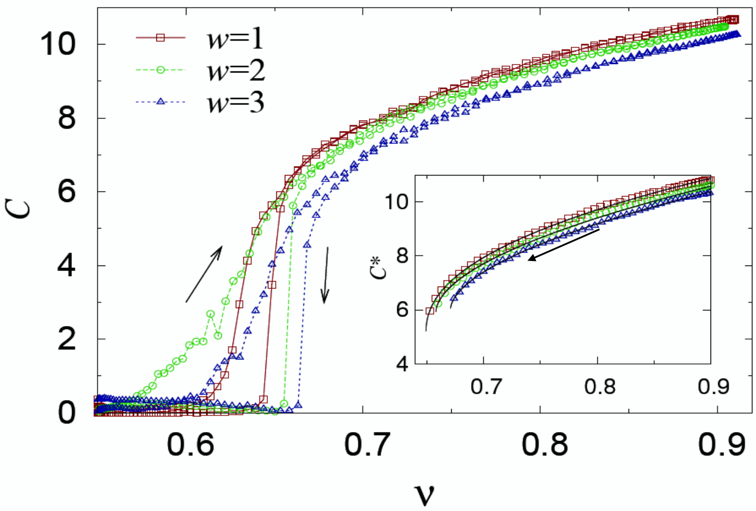
$\nu_{N=10000} = 0.6652$

Coordination number – Effect of polydispersity

- Uniform radius distribution
- $w = r_{max}/r_{min}$



Coordination number – Effect of polydispersity

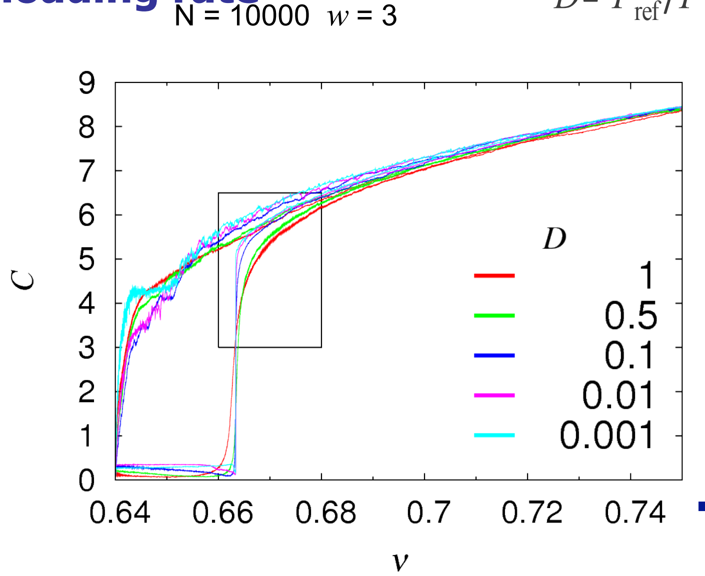


$\nu_{w=1} = 0.649$

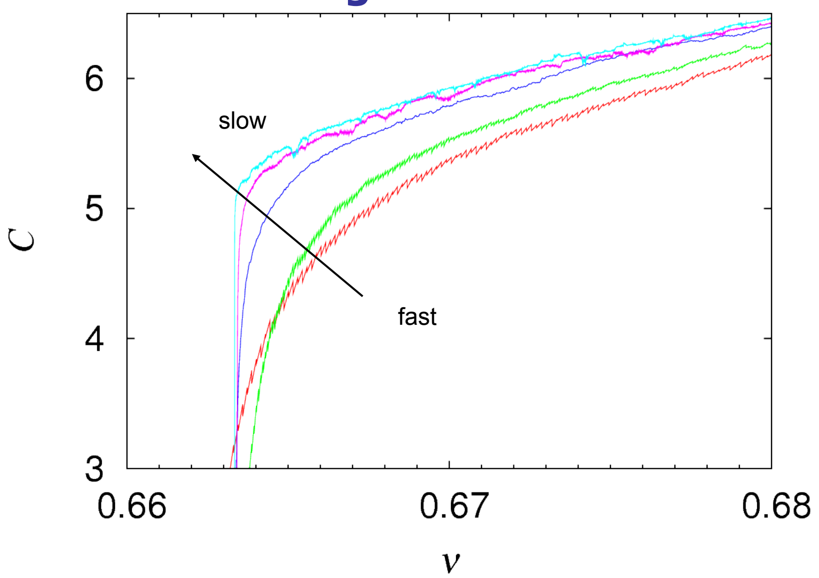
$\nu_{w=2} = 0.658$

$\nu_{w=3} = 0.671$

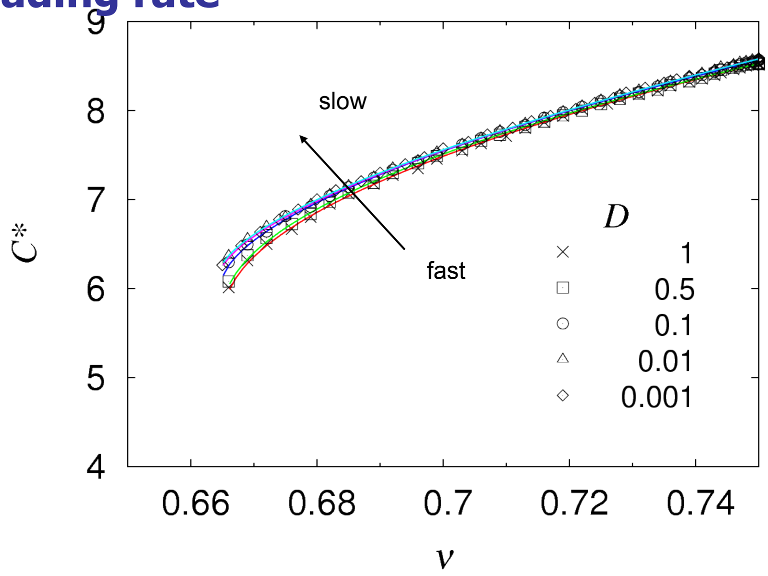
Coordination number – Effect of loading rate



Coordination number
Effect of loading rate

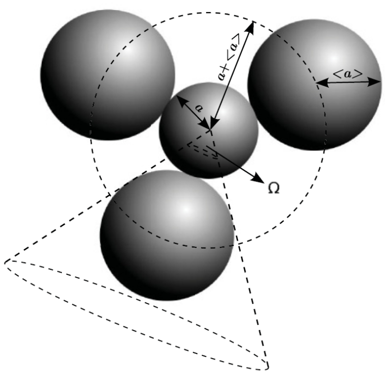


Coordination number – Effect of loading rate



Coordination number – Analytical model

Assumption: neighbor particles are identical with radius <r>



Solid angle

$$\Omega(r) = 2\pi\left(1 - \frac{\sqrt{(r+\langle r\rangle)^2 - \langle r\rangle}}{r+\langle r\rangle}\right)$$

$$C(r) = \frac{4\pi c_s}{\Omega(r)},$$

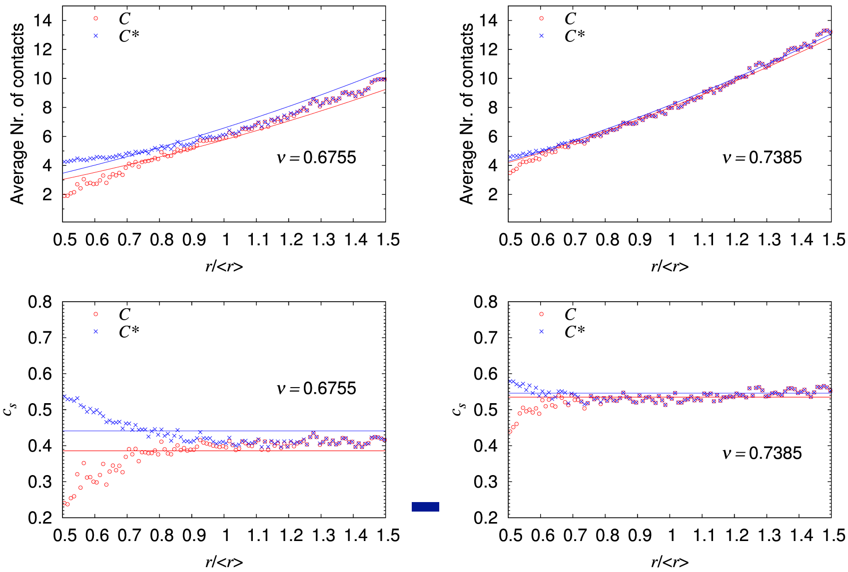
$$C = \int_0^\infty C(r) f(r)\,dr$$

$$= 4\pi c_s \int_0^\infty [f(r)/\Omega(r)]dr$$

Compactity c_s (total fraction of shielded surface) is constant

Shaebani et al. PRE 2012 and references therein

Distribution of contacts and Compacity



Trace of fabric

$$\mathbf{F} = \langle \mathbf{F}^p \rangle = \frac{1}{V} \sum_{p \in V} w_V^p V^p \sum_{c=1}^{C^p} \mathbf{n}^c \otimes \mathbf{n}^c$$

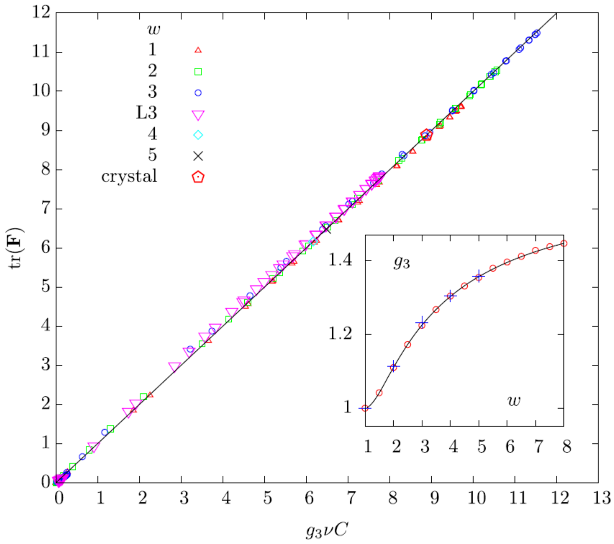
$$\begin{aligned} \mathrm{tr}(\mathbf{F}) &= (1/V) \sum_{p \in V} V_p C_p \\ &= (N/V) \int_0^\infty dr\, V_p(r) C(r) f(r) \\ &= g_3 \nu C \ , \end{aligned}$$

$$g_3 = \frac{\langle r^3 \rangle_\Omega}{\langle r^3 \rangle} = \frac{\int_0^\infty r^3 [f(r)/\Omega(r)]\, dr}{\langle r^3 \rangle \int_0^\infty [f(r)/\Omega(r)]\, dr} \ ,$$

$$g_3 \approx \frac{1 - B_2 + C_2 + (B_2 - 2C_2) \frac{\langle r^4 \rangle}{\langle r \rangle \langle r^3 \rangle} + C_2 \frac{\langle r^5 \rangle}{\langle r \rangle^2 \langle r^3 \rangle}}{1 + C_2 \left[\frac{\langle r^2 \rangle}{\langle r \rangle^2} - 1 \right]}$$

$a_2 = \Omega(\langle r \rangle)/(4\pi) = \frac{1}{2}\left(1 - \sqrt{3}/2\right)$,
$B_2 = \sqrt{3}/24 a_2$, and
$C_2 = B_2 (B_2 - 5/6)$

Trace of fabric



Constitutive model for Pressure

Micromechanical stress tensor for a particle

$$\sigma^p_{ij} = \frac{1}{V_p} \sum_{c=1}^{C_p} l_i^{pc} f_j^{pc} \,, \qquad \mathbf{l}^{pc} = (r_p - \delta_c/2)\hat{\mathbf{n}} \qquad \mathbf{f}^{pc} = k_n \delta_c \hat{\mathbf{n}}$$

- Branch vector
- Contact force

$$\mathrm{tr}(\boldsymbol{\sigma}^p) = \frac{k_n}{V_p} \sum_{c=1}^{C_p} \delta_c \left(r_p - \frac{\delta_c}{2} \right)$$

$$\mathrm{tr}(\boldsymbol{\sigma}) = \frac{1}{V} \sum_{p \in V} V_p \, \mathrm{tr}(\boldsymbol{\sigma}^p)$$

$$= \frac{k_n}{V} \sum_{p=1}^{N} \left(r_p \sum_{c=1}^{C_p} \delta_c - \frac{1}{2} \sum_{c=1}^{C_p} \delta_c^2 \right) \,,$$

Constitutive model for Pressure

Average pressure in a packing:

$$\mathrm{tr}(\boldsymbol{\sigma}) = \frac{3k_n\nu}{4\pi\langle r^3\rangle}\,\frac{1}{N}\sum_{p=1}^{N}\left(r_p\sum_{c=1}^{C_p}\delta_c - \frac{1}{2}\sum_{c=1}^{C_p}\delta_c^2\right)$$

$$= \frac{3k_n}{4\pi}\,\frac{\nu}{\langle r^3\rangle}\left(\langle\sum_{c=1}^{C_p}\delta_c\rangle\langle r_p\phi_p\rangle - \frac{1}{2}\langle\sum_{c=1}^{C_p}\delta_c^2\rangle\right)$$

$$= \frac{3k_n}{4\pi}\,\frac{\nu C\langle\delta\rangle_c}{\langle r^3\rangle}\left(\langle r_p\phi_p\rangle - \frac{\langle\delta^2\rangle_c}{2\langle\delta\rangle_c}\right)$$

Normalized contact force

$$\phi_p \equiv f_p/\langle f_p\rangle, \text{ with } f_p = \textstyle\sum_{c=1}^{C_p} k_n\delta_c$$

$$C = \frac{M_4}{N} = \frac{1}{N}\textstyle\sum_{p\in N_4} C_p \qquad \langle\delta\rangle_c \equiv \frac{1}{M_4}\sum_{c\in M_4}\delta_c$$

Constitutive model for Pressure

Dimensionless pressure

$$p = p(\langle\Delta\rangle_c) = \frac{1}{4\pi}\nu C\langle\Delta\rangle_c\left(2g_p - b\langle\Delta\rangle_c\right)\ ,$$

$$g_p = \frac{\langle\xi_p\phi_p\rangle}{\langle\xi^3\rangle} \quad \text{and} \quad b = \frac{1}{\langle\xi^3\rangle}\,\frac{\langle\Delta^2\rangle_c}{\langle\Delta\rangle_c^2}\ .$$

$$\xi_p = r_p/\langle r\rangle$$
$$\Delta_c = \delta_c/\langle r\rangle$$

$$g_p = 1 \quad \text{if} \quad w = 1$$

$$g_p = \frac{1}{\langle\xi^3\rangle}\int_0^\infty \xi\phi(\xi)h(\xi)\,\mathrm{d}\xi \quad \text{else}$$

Constitutive model for Pressure

Linking particle overlap and macroscopic deformation

$$\mathrm{d}\delta = n_i \mathrm{d}l_i = \langle r \rangle \, n_i u_{i,j} n_j$$

$$\mathrm{d}\langle \Delta \rangle_c = D\epsilon_{\mathrm{v}}$$

$$\epsilon_{\mathrm{v}} = \mathrm{tr}(\epsilon_{\mathrm{ij}})$$

$$\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$$

Assumption:
for small overlaps the length of the branch vector is equal to the average particle radius

Off diagonal terms of strain tensor vanish because isotropic deformation and contact distribution

$$\langle \Delta \rangle_c = D \int_{V_0}^{V} \epsilon_{\mathrm{v}} = D\varepsilon_{\mathrm{v}} = D \ln\left(\frac{\nu_c}{\nu}\right)$$

Constitutive model for Pressure

$$p = p_0 \frac{\nu C}{\nu_c}(-\varepsilon_{\mathrm{v}})\left[1 - \gamma_p(-\varepsilon_{\mathrm{v}})\right]$$

$$B = -V(\partial p/\partial V) = \partial p/\partial(-\varepsilon_{\mathrm{v}}) = \nu \partial p/\partial \nu$$

$$B = \frac{\partial p}{\partial(-\varepsilon_{\mathrm{v}})} = \frac{p_0 F_V}{g_3 \, \nu_c}\left[1 - 2\gamma_p(-\varepsilon_{\mathrm{v}}) + (-\varepsilon_{\mathrm{v}})\left[1 - \gamma_p(-\varepsilon_{\mathrm{v}})\right]\frac{\partial \ln(F_V)}{\partial(-\varepsilon_{\mathrm{v}})}\right]$$

$$F_V = \mathrm{tr}(\mathbf{F}) = g_3 \nu C$$

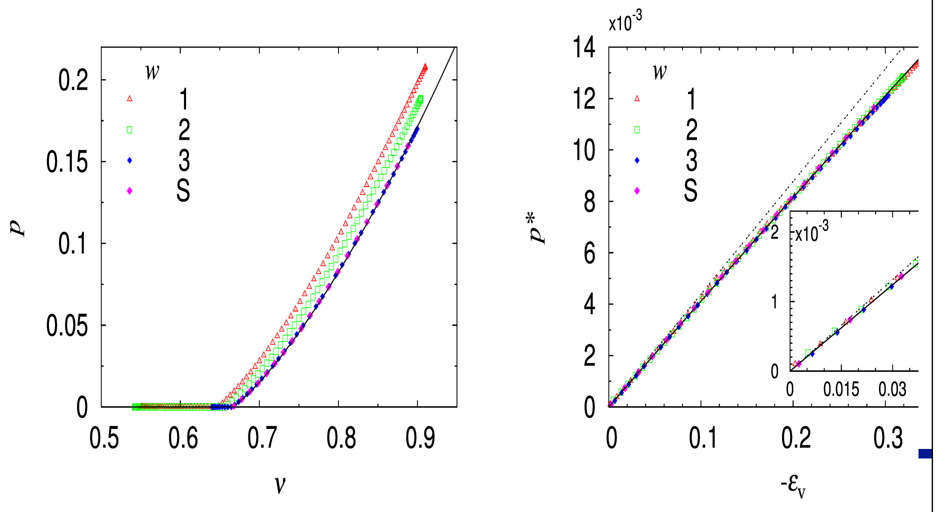
Evolution Equation(s):

$$\mathrm{d}p = B(-\mathrm{d}\varepsilon_{\mathrm{v}})$$

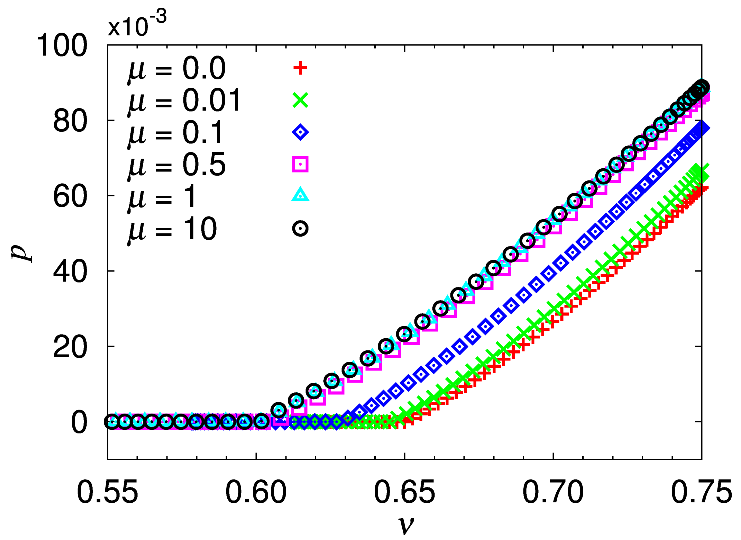
$$\mathrm{d}F_V = F_V\left(1 + \nu\frac{\partial C}{\partial \nu}\right)(-\mathrm{d}\varepsilon_{\mathrm{v}})$$

Isotropic compression – Pressure

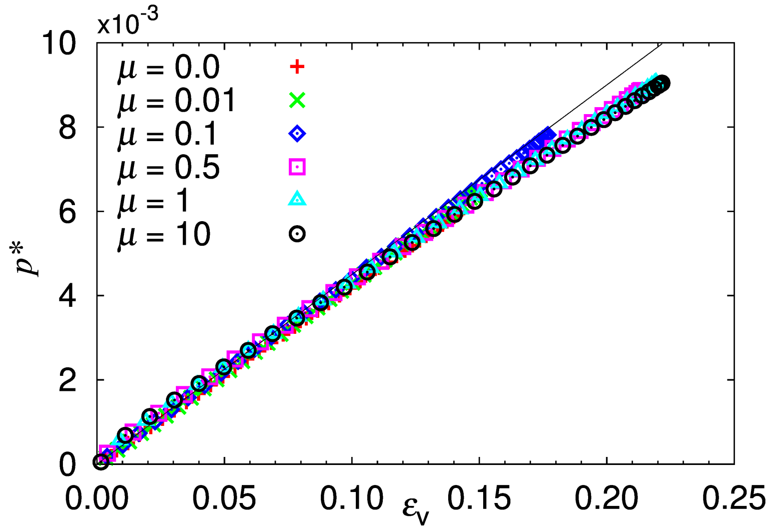
$$p = p_0 \frac{\nu C}{\nu_c}(-\varepsilon_v)\,[1-\gamma_p(-\varepsilon_v)] \qquad p^* = \frac{p\nu_c}{\nu C} = p_0(-\varepsilon_v)\,[1-\gamma_p(-\varepsilon_v)]$$



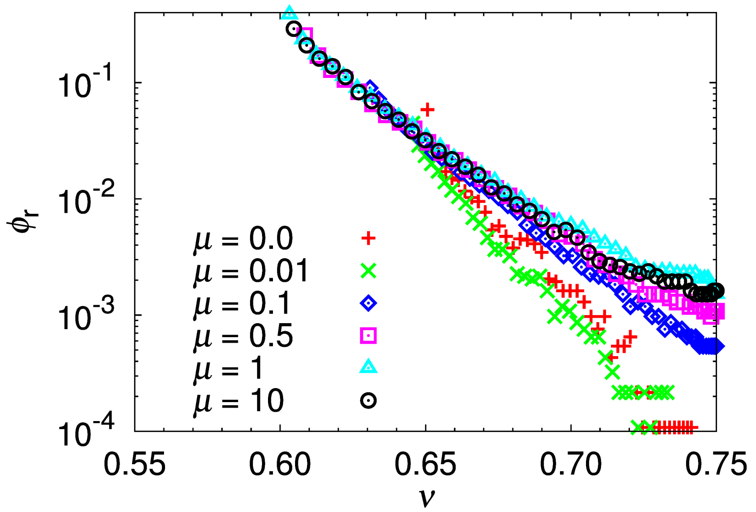
Isotropic compression – Effect of friction



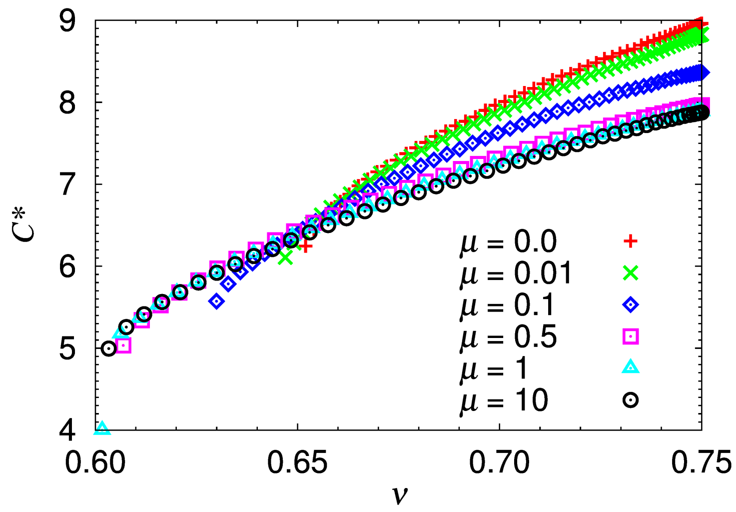
Isotropic compression – Effect of friction



Isotropic compression
Effect of friction – Rattlers



Isotropic compression
Effect of friction – Coordination number



Constitutive model – isotropic (mode 0)
scalar! (in the biaxial box eigen-system)

Isotropic stress $\delta\sigma_V = 2B\varepsilon_V$

Deviatoric stress $\delta\tau = A\varepsilon_V$

Anisotropy $\delta A = 0$

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

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

Constitutive model
various deformation modes

Mode 0: Isotropic $d\gamma = 0$

Mode 1: Uni-axial

Mode 2: Deviatoric $\varepsilon_V = 0$

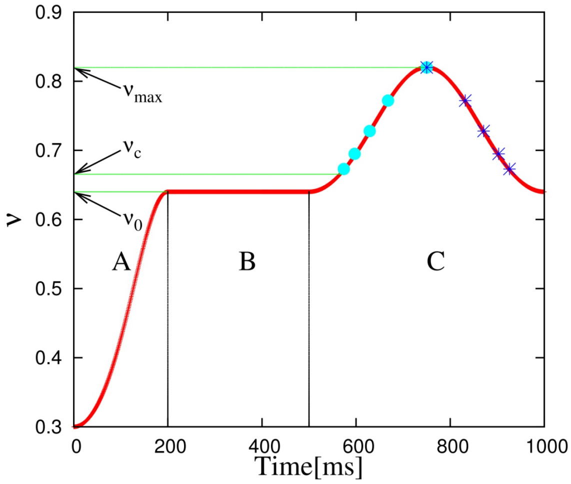
Mode 3: Bi-axial (side-stress controlled)

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

Sample preparation

Isotropic Compression

$$\varepsilon^{ISO}_{-1,-2,-3} = \begin{bmatrix} -\varepsilon_0 & 0 & 0 \\ 0 & -\varepsilon_0 & 0 \\ 0 & 0 & -\varepsilon_0 \end{bmatrix}$$



O. I. Imole et al., KONA, 2013

Deformation Modes

UNI

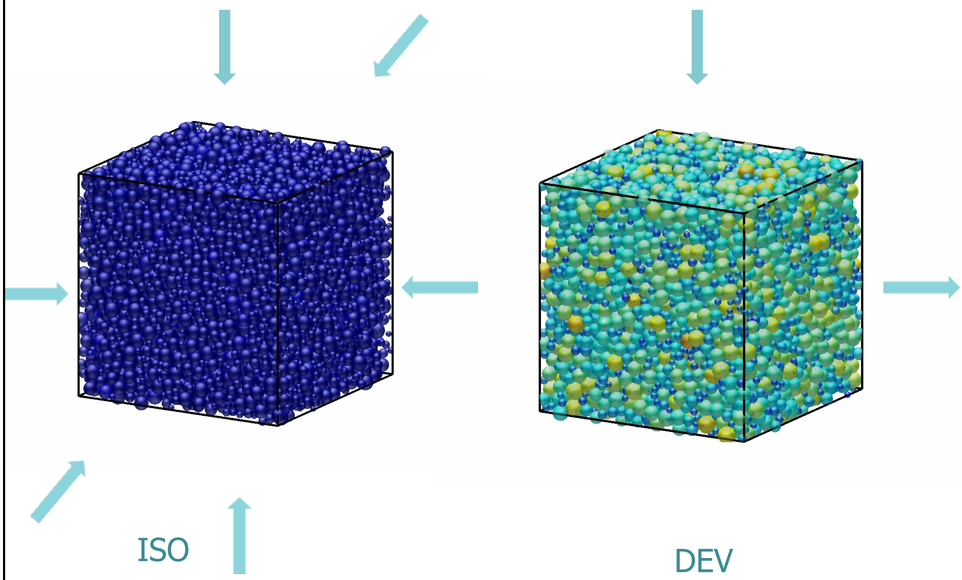
$$\varepsilon^{UNI}_{0,0,-1} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\varepsilon_0 \end{bmatrix}$$

DEV 2

$$\varepsilon^{D2}_{1,0,-1} = \begin{bmatrix} \varepsilon_0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\varepsilon_0 \end{bmatrix}$$

DEV 3

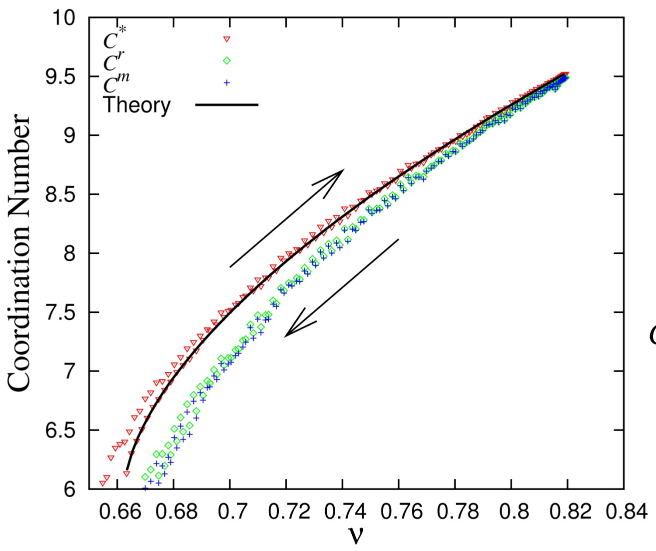
$$\varepsilon^{D3}_{1/2,1/2,-1} = \begin{bmatrix} 1/2\varepsilon_0 & 0 & 0 \\ 0 & 1/2\varepsilon_0 & 0 \\ 0 & 0 & -\varepsilon_0 \end{bmatrix}$$



Movie time!

Microscopic quantities – Coordination Number

Uniaxial



$$C^r = \frac{M}{N}$$

$$C^m = \frac{M_4}{N}$$

$$C^* = \frac{M_4}{N_4}$$

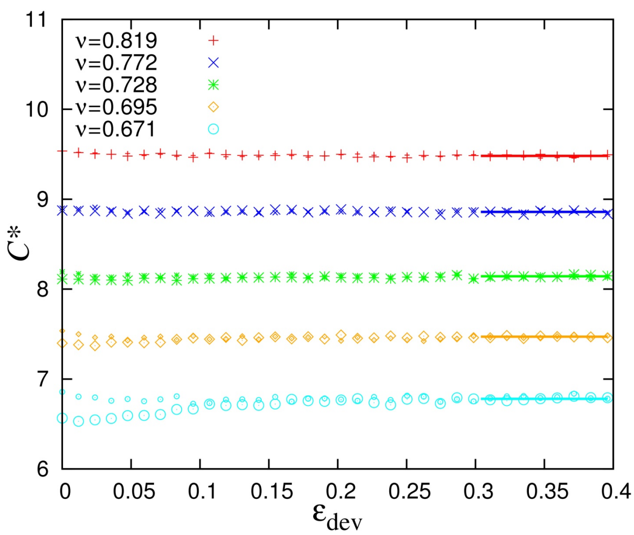
$$C^*(\nu) = C_0 + C_1\left(\frac{\nu}{\nu_c} - 1\right)^{\alpha}$$

$(C^r \approx C^m) < C^*$

F. Göncü et al. C.R. Mecanique 338:10-11 (2010)

Microscopic quantities – Coordination Number

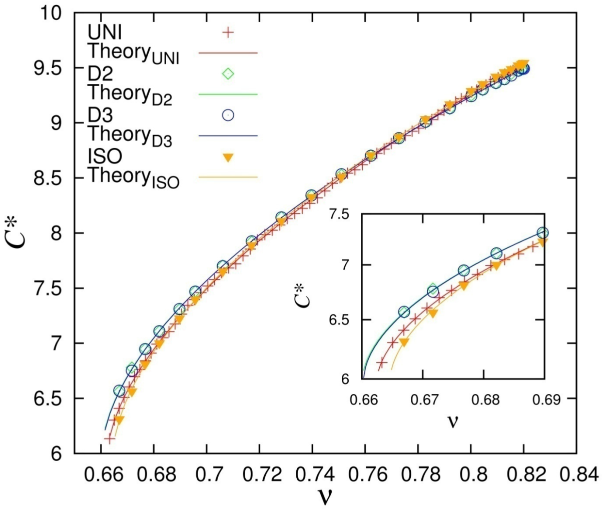
DEV2



$$C^* = \frac{M_4}{N_4}$$

Microscopic quantities – Coordination Number

All modes



$$C^* = \frac{M_4}{N_4}$$

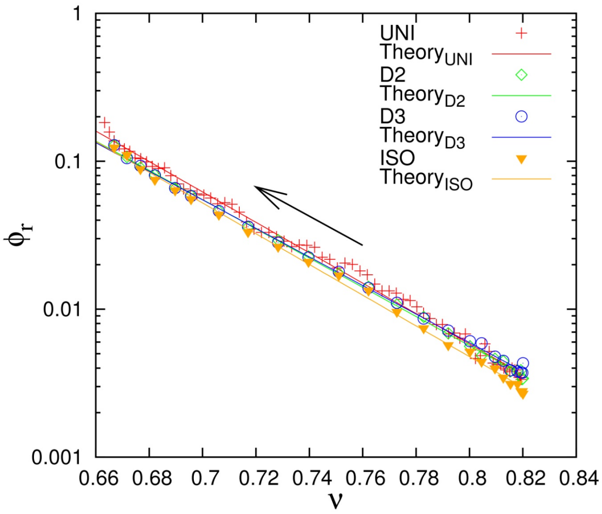
$$C^*(v) = C_0 + C_1\left(\frac{v}{v_c} - 1\right)^{\alpha}$$

- Deviatoric deformation reduce the jamming point of a dense packing

- ISO leads to higher jamming point after unloading

ISO > UNI > DEV

Fraction of Rattlers



$$\phi_r(v) = \phi_c \exp\left[-\phi_v\left(\frac{v}{v_c} - 1\right)\right]$$

- Strongest difference at higher volume fraction

-Lower during isotropic unloading

-Higher during uniaxial unloading (almost 20% at the end of unloading)

Macroscopic quantities

Static Stress Tensor $\sigma_{\alpha\beta} = \frac{1}{V}\sum_{c\in V} f_\alpha^c l_\beta^c$

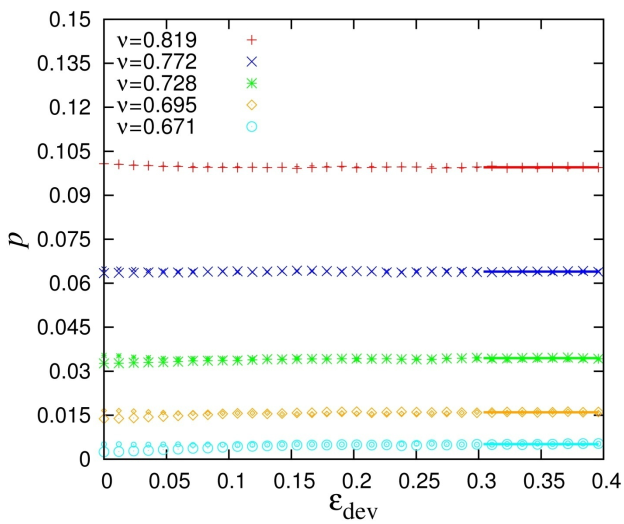
Pressure $P = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$

Non-Dimensional Pressure $p = \frac{2 < r >}{3k_n} tr(\sigma)$

Deviatoric Stress $\sigma_{dev} = \sqrt{\frac{(\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{xx} - \sigma_{zz})^2 + (\sigma_{yy} - \sigma_{zz})^2}{2}}$

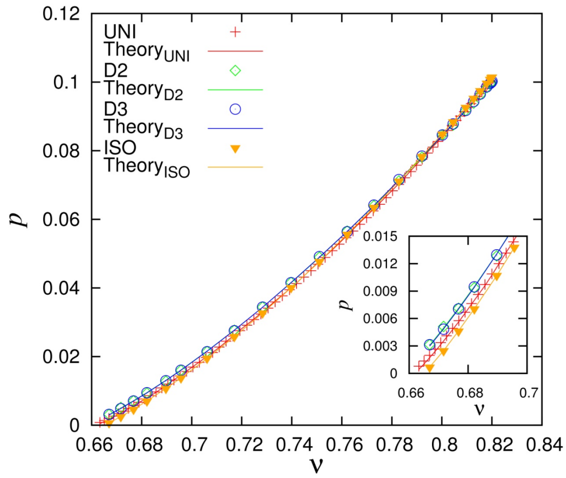
Deviatoric Strain $\varepsilon_{dev} = \sqrt{\frac{(\varepsilon_{xx} - \varepsilon_{yy})^2 + (\varepsilon_{xx} - \varepsilon_{zz})^2 + (\varepsilon_{yy} - \varepsilon_{zz})^2}{2}}$

Non-Dimensional Pressure



DEV 2

Non-Dimensional Pressure

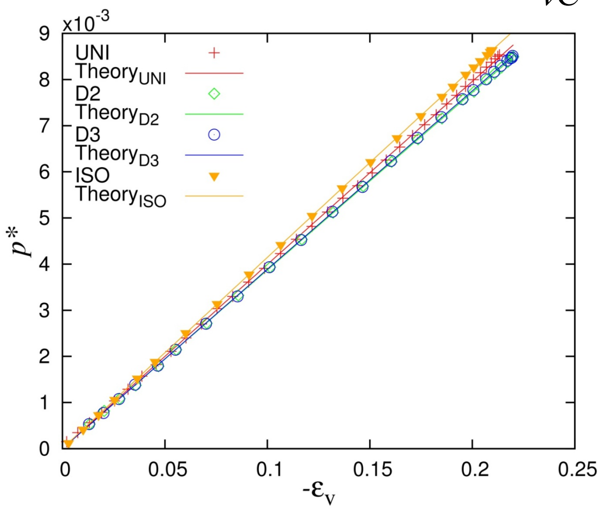


- Data collapse on a unique law at high volume fraction

- Slight divergence at low volume fraction due to difference in the critical volume fraction

Scaled Pressure

$$p^* = \frac{p v_c}{\nu C} = p_0(-\varepsilon_v)[1 - \gamma_p(-\varepsilon_v)]$$



- Data collapse on a unique law at low volume fraction

-At high volume fraction, ISO > UNI > DEV

$$\varepsilon_v = -\ln\left(\frac{\nu}{\nu_c}\right)$$

Table of Parameters

C^*	C_1	α	ν_c
ISO_G	8.0 ± 0.5	0.58 ± 0.05	0.66 ± 0.01
ISO	8.2720	0.5814	0.6646
UNI	8.3700	0.5998	0.6625
D2	7.9219	0.5769	0.6601
D3	7.9289	0.5764	0.6603

ϕ_r	ϕ_c	ϕ_v
ISO_G	0.13 ± 0.03	15 ± 2
ISO	0.1216	15.8950
UNI	0.1507	15.6835
D2	0.1363	15.0010
D3	0.1327	14.6813

p^*	p_0	γ_p	ν_c
ISO_G	0.04180	0.11000	0.6660
ISO	0.04172	0.06228	0.6649
UNI	0.04006	0.03270	0.6619
D2	0.03886	0.03219	0.6581
D3	0.03899	0.02819	0.6583

O. I. Imole et al., KONA, 2013

Qualitatively and quantitatively:

Isotropic quantities are controlled by isotropic strain
Deviatoric quantities (see below) by deviatoric strain

Jamming density is a state variable!
dependent on the deformation mode

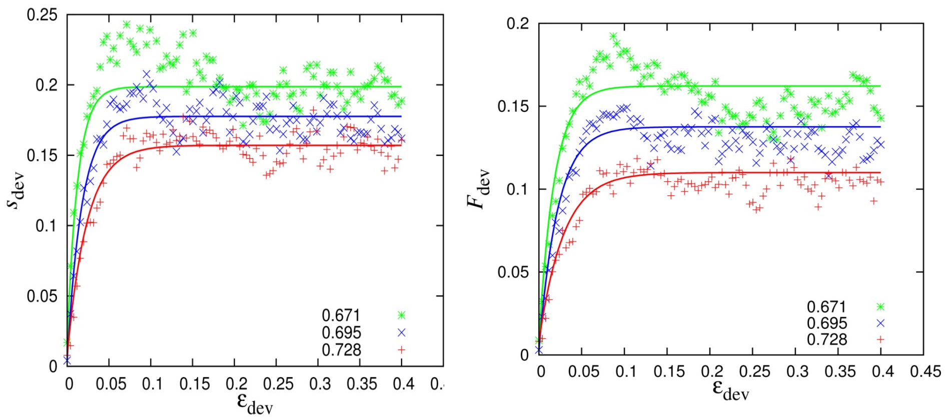
Scales all isotropic data ☺

Theory

Macroscopic Evolution Equations

Deviatoric Stress Ratio

$$s_{dev} = \frac{\sigma_{dev}}{p}$$



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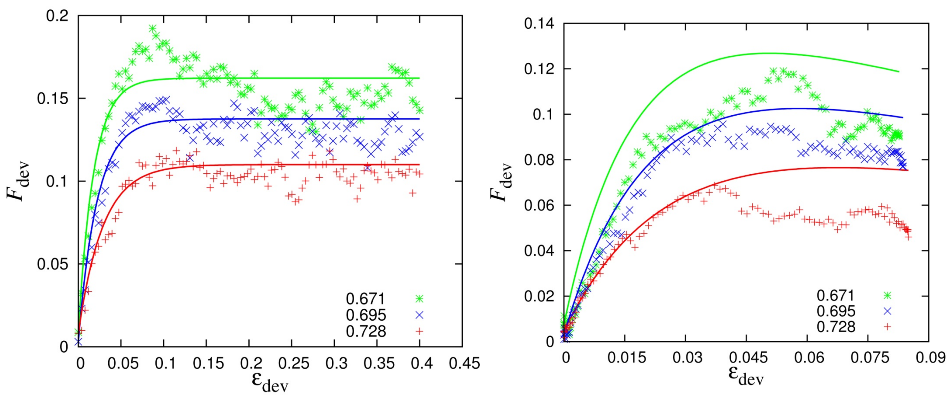
Calibration DEV2

Deviatoric Fabric



O. I. Imole et al., KONA, 2013

Calibration DEV2

The Anisotropy Model

Generalized for a $\mathcal{D}$ −dimensional system

$$\delta P = \mathcal{D} B \delta\epsilon_{\mathrm{v}} + A S \delta\epsilon_{\mathrm{dev}},$$
$$\delta\sigma_{\mathrm{dev}} = A \delta\epsilon_{\mathrm{v}} + \mathcal{D} G^{\mathrm{oct}} S \delta\epsilon_{\mathrm{dev}},$$
$$\delta A = \beta_A \,\mathrm{sign}\,(\delta\epsilon_{\mathrm{dev}})(A^{\max} - A)\delta\epsilon_{\mathrm{dev}}.$$

$S = (1 - s_{\mathrm{dev}}/s_{\mathrm{dev}}^{\max})$ Stress-Isotropy

β_A is the growth rate of A

$A^{\max}$ represents the maximum anisotropy

G^{oct} is octahedral shear modulus

Luding and Perdahcioglu CIT (2011), Magnanimo and Luding GM (2011), Imole et al. KONA (2013)

Reduced Theoretical Model

- Model parameters as functions of ν from various deviatoric simulations

Assumptions :

- Macroscopic field A is proportional to the microscopic rank-two deviatoric fabric F_{dev} $\boldsymbol{\beta_F = \beta_A}$
- Both A and s_{dev} approach their limit states exponentially fast
- Only one anisotropy modulus A is sufficient (valid in 2D, questionable in 3D, possibly two moduli A_1 and A_2 are needed)

Reduced Theoretical Model

Deviatoric Stress

$$s_{\text{dev}} = s_{\text{dev}}^{\max} - \left(s_{\text{dev}}^{\max} - s_{\text{dev}}^{0}\right) e^{-\beta_s \epsilon_{\text{dev}}},$$

$-$ s_{dev}^{0} and $s_{\text{dev}}^{\max}$ represent the initial and maximum values of s_{dev}

$-$ β_s is its growth rate

Deviatoric Fabric

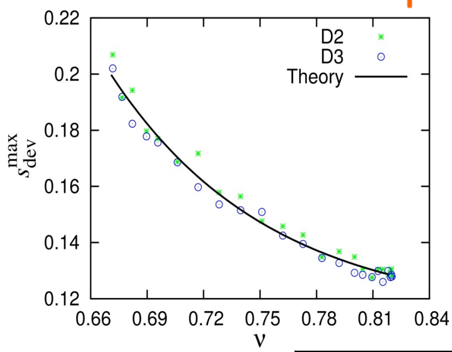
$$F_{\text{dev}} = F_{\text{dev}}^{\max} - \left(F_{\text{dev}}^{\max} - F_{\text{dev}}^{0}\right) e^{-\beta_F \epsilon_{\text{dev}}}$$

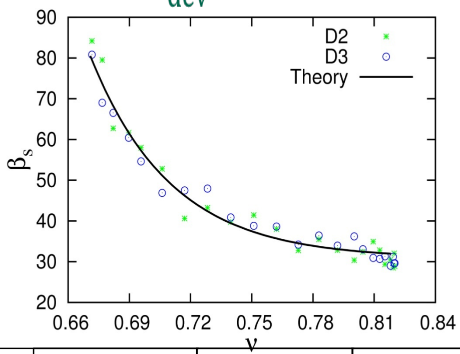
$-F_{\text{dev}}^{0}$ and $F_{\text{dev}}^{\max}$ represent the initial and maximum (saturation) values of the deviatoric fabric

$-\beta_F$ is its rate of change

$$A \approx a_0^* F_{\text{dev}} \frac{P \nu_c^2}{(\nu - \nu_c)} \approx \frac{a_0 k}{2\langle r \rangle} F_\nu F_{\text{dev}}$$

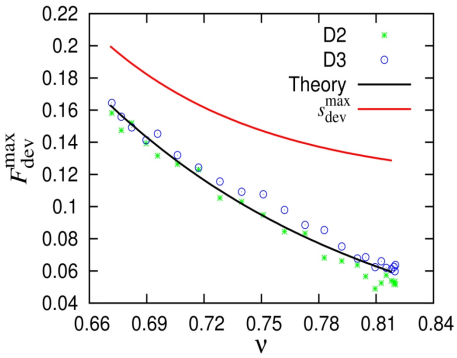
Calibration of model parameters - s_{dev}

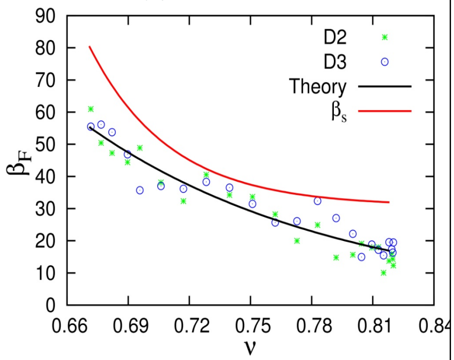




Evolution Parameters	Q_{max}	Q_v	α
s_{dev}^{max}	0.1137	0.09166	7.916
β_s	30.76	57.00	16.86

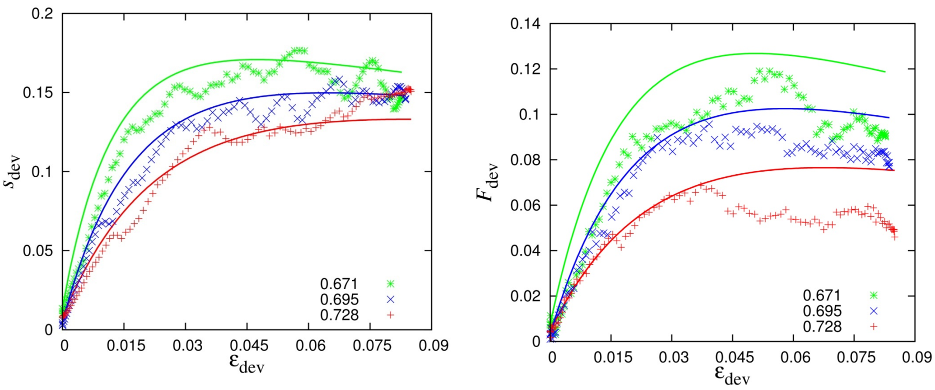
Calibration of model parameters - F_{dev}



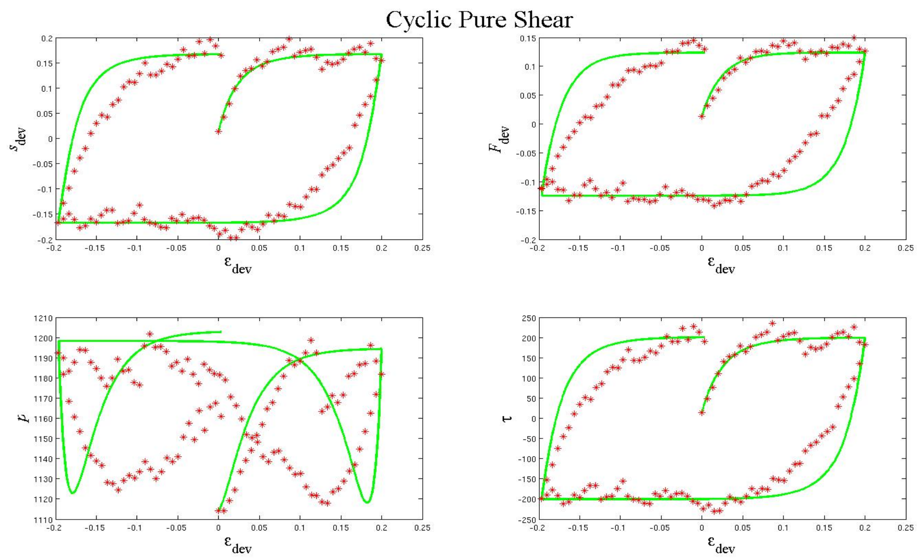


Evolution Parameters	Q_{max}	Q_v	α
F_{dev}^{max}	0	0.1694	4.562
β_F	0	57.89	5.366

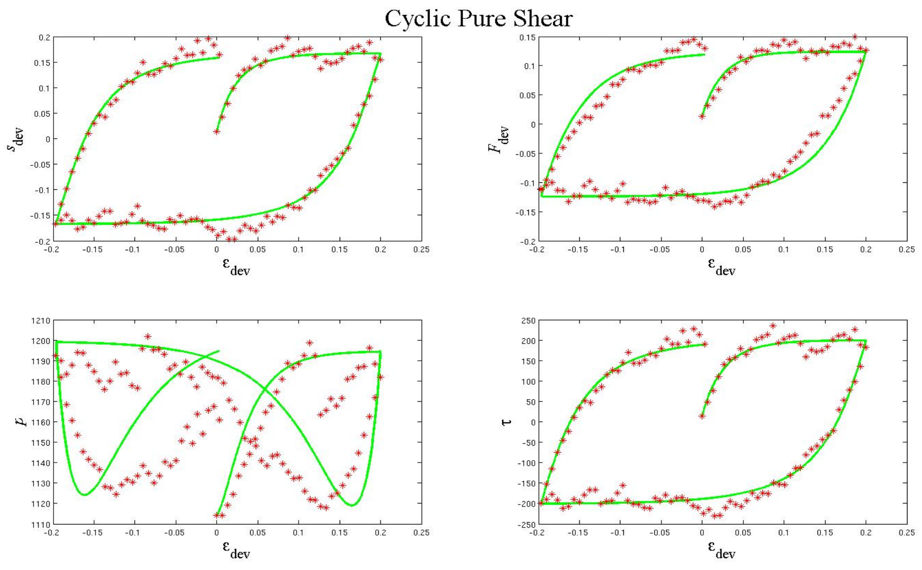
Prediction: Uniaxial



Prediction: Cyclic Shear



Prediction (improved model) – Cyclic Shear



Conclusions

- Corrected coordination number (without rattlers) well predicted by an analytical equation

- Jamming volume fraction depends on deformation mode! (Over-compression leads to higher volume fraction. Differences pronounced at lower volume fractions.)

- Scaled pressure linear in strain!!! + perturbation. Uniaxial and deviatoric data deviate from isotropic only at large strain.

- Uniaxial and cyclic modes well predicted by the anisotropy model calibrated with D2 and D3 modes.