Micro-macro transition, simple examples

Stefan Luding
PART/DCT, TUDelft, NL

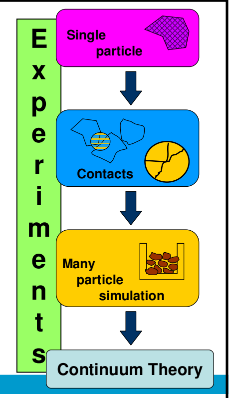
Special thanks to: M. Lätzel (Stuttgart)

Stefan Luding, s.luding@tnw.tudelft.nl
Particle Technology, DelftChemTech, Julianalaan 136, 2628 BL Delft

TUDelft
Delft University of Technology

Micro-Macro Approach

- Introduction
  - single particles
  - many particle systems
  - continuum theory



Why ?

- `Many particle' simulations work for small systems only (10^4- 10^6)
- Industrial scale applications rely on FEM
- FEM relies on continuum mechanics + constitutive relations
- `Micro-macro' can provide those !
- Homogenization/Averaging

Why constitutive relations ?

Static equilibrium (particles)

$$\sum_{c=1}^{C} \vec{f}^c = 0$$

DN equations, $CN/2$ contacts
1 (unknown) force per contact
$\Rightarrow C=2D$ (frictionless, isostatic)

Static equilibrium (cont.-theory)

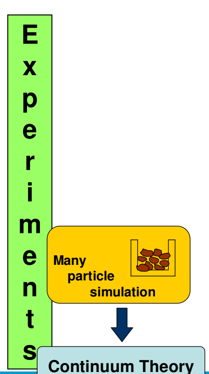
$$\mathrm{div}\ \boldsymbol{\sigma} = 0 \rightarrow \begin{cases} \partial_x \sigma_{xx} + \partial_z \sigma_{xz} = 0 \\ \partial_x \sigma_{zx} + \partial_z \sigma_{zz} = 0 \end{cases}$$

D equations
$D(D+1)/2$ unknowns
$\Rightarrow$ 1 eq. missing (2D)

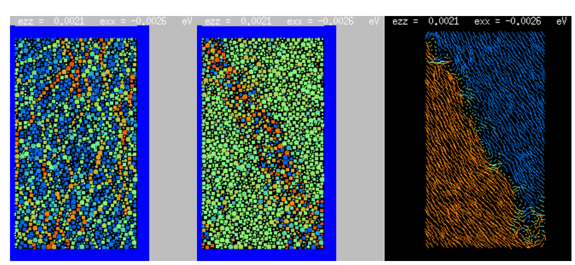
... missing constitutive equation(s)

Micro-Macro Approach

- Introduction
- Homogenization+Averaging
  - Scalars
  - Vectors
  - Tensors
- Rotations+Averaging
- Conclusion



Micro informations: shear bands



potential energy rotations displacements

Literature

[5] S. Luding, *Micro-macro transition for an-isotropic, frictional granular packings,* Int. J. Sol. Struct. 41(21), pp. 5821-5836, 2004, http://www.ica1.uni-stuttgart.de/~lui/PAPERS/mmshort4.pdf

[6] S. Luding, *Micro-Macro Models for Anisotropic Granular Media*, in: Modelling of Cohesive-Frictional Materials, P. A. Vermeer, W. Ehlers, H. J. Herrmann, E. Ramm, eds., Balkema, Leiden, 2004 (ISBN 04 1536 023 4), pp. 195-206 http://www.ica1.uni-stuttgart.de/~lui/PAPERS/cdm2004_luding.pdf

[7] M. Lätzel, S. Luding, H. J. Herrmann, D. W. Howell, and R. P. Behringer, *Comparing Simulation and Experiment of a 2D Granular Couette Shear Device,* Eur. Phys. J. E 11, 325-333, 2003, http://www.ica1.uni-stuttgart.de/~lui/PAPERS/shear_simexp.pdf

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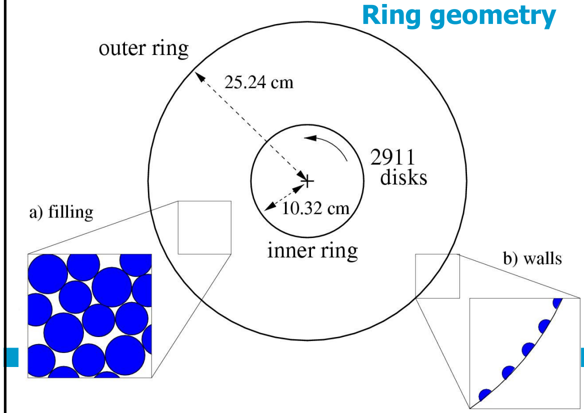
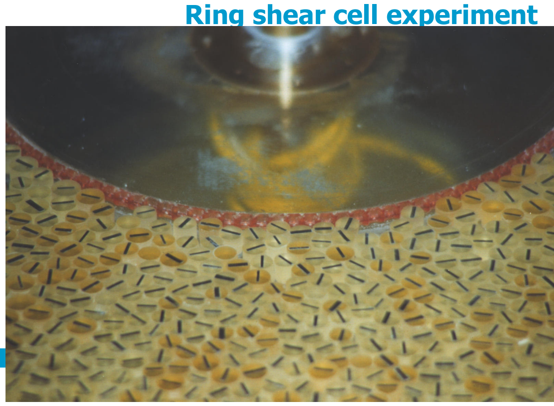
[9] S. Luding, M. Lätzel, and H. J. Herrmann, *From discrete element simulations towards a continuum description of particulate solids*, in: Handbook of Conveying and Handling of Particulate Solids, Elsevier, Netherlands, 39--44, 2001, http://www.ica1.uni-stuttgart.de/~lui/PAPERS/israel1.pdf

[10] M. Lätzel, S. Luding, and H. J. Herrmann, *Macroscopic material properties from quasi-static, microscopic simulations of a two-dimensional shear-cell*, Granular Matter 2(3), 123-135, 2000 http://www.ica1.uni-stuttgart.de/~lui/PAPERS/micmac.pdf

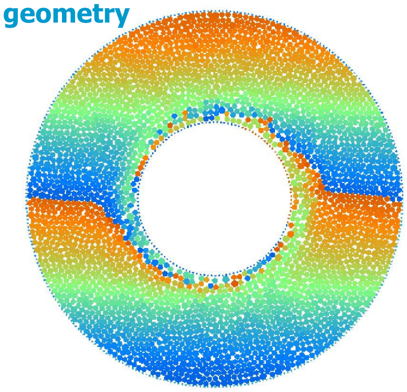
Ring geometry



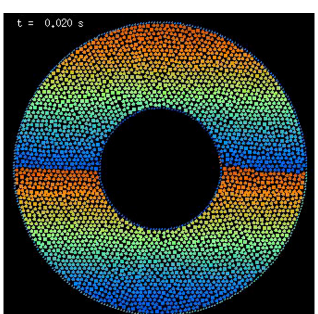
Ring shear cell experiment



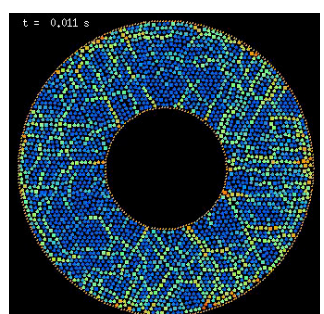
Ring geometry



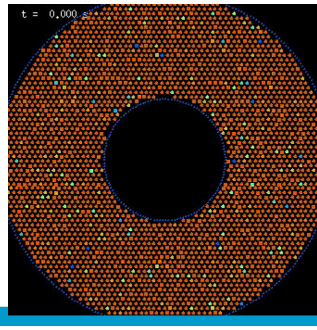
2D shear cell – shear band



2D shear cell – force chains



2D shear cell – energy



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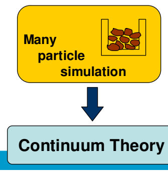
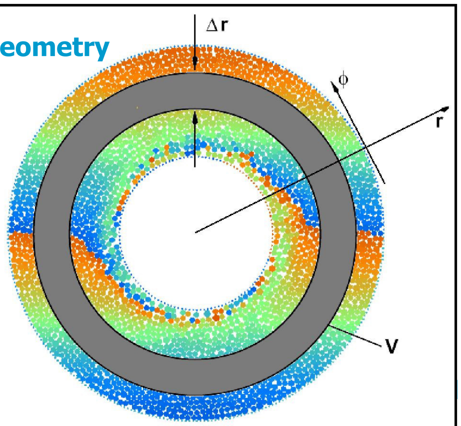


Ring geometry



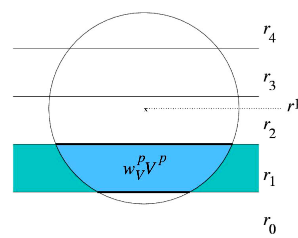
Averaging Formalism

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

Any quantity:

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

- Scalar
- Vector
- Tensor



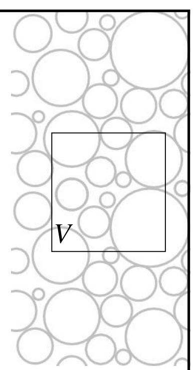
Averaging Formalism

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

Any quantity:

$$Q^p$$

In averaging volume: V



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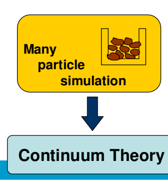


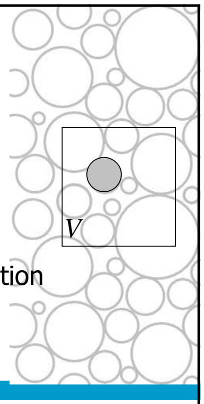
Averaging Density

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

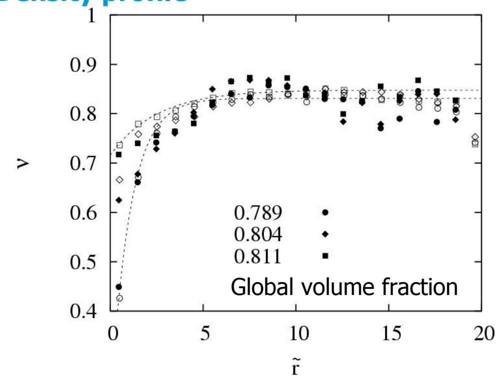
Any quantity:

$$Q^p = 1$$

- Scalar: Density/volume fraction



Density profile



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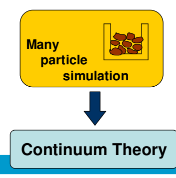


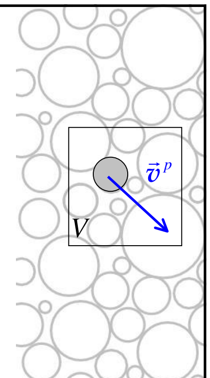
Averaging Velocity

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

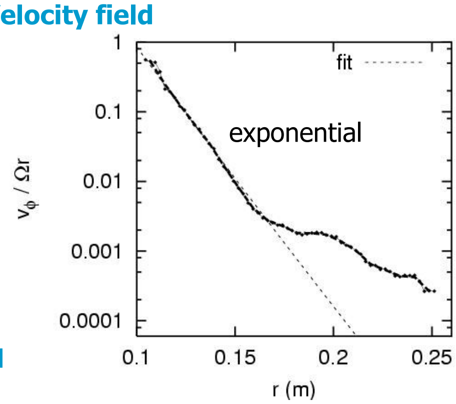
Any quantity:

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

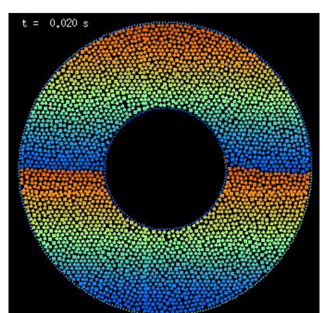
- Scalar
- Vector – velocity density



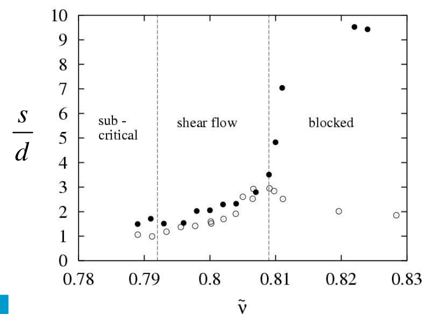
Velocity field



2D shear cell – shear band



Velocity gradient $\nabla \mathbf{v} \;\; \rightarrow \;\; D_{r\phi} = \frac{1}{2}\left[\frac{\partial v_\phi}{\partial r} - \frac{v_\phi}{r}\right]$



exponential: $v_\phi(r) = v_0 \exp(-(r - R_i)/s)$

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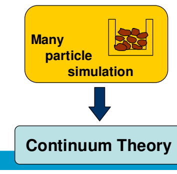


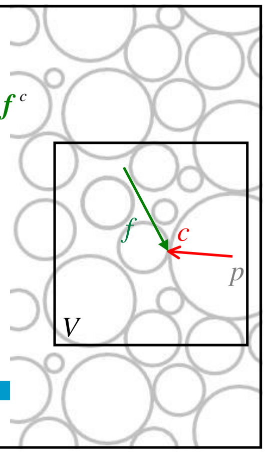
Averaging Stress

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

Any quantity:

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

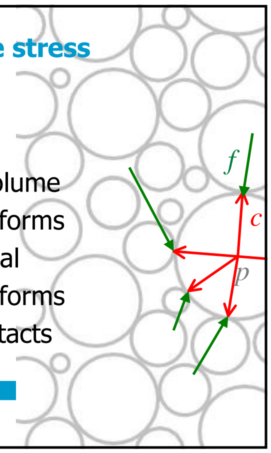
- Scalar
- Vector
- Tensor: Stress



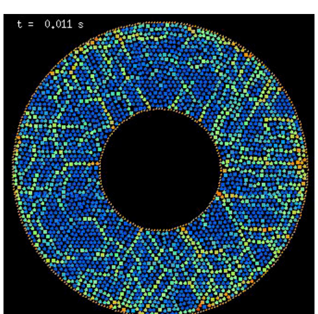
Derive single particle stress

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

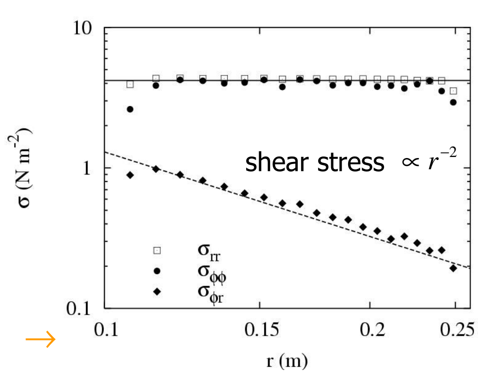
Av. stress over pp.-volume
Volume integral transforms to surface integral
Surface integral transforms to sum over contacts



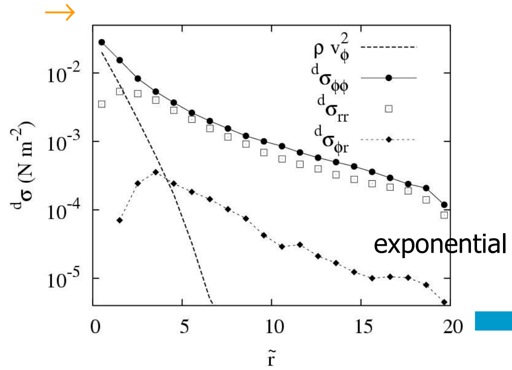
2D shear cell – force chains



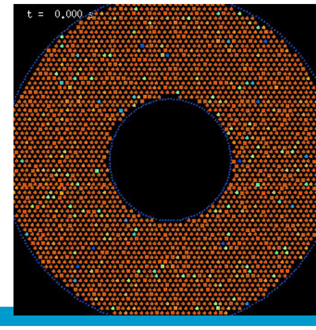
Stress tensor (static)



Stress tensor (dynamic)



2D shear cell – energy



Stress equilibrium (1)

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

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

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

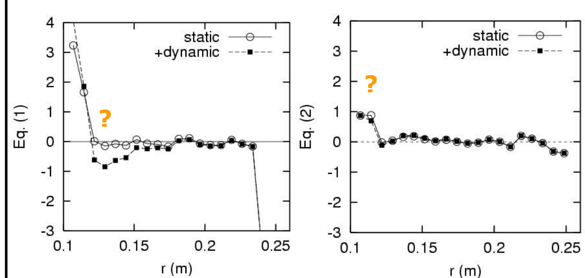
$$0 = r\frac{\partial\sigma_{r\phi}}{\partial r} + (\sigma_{r\phi} + \sigma_{\phi r}),$$

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

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

Stress equilibrium (2)

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



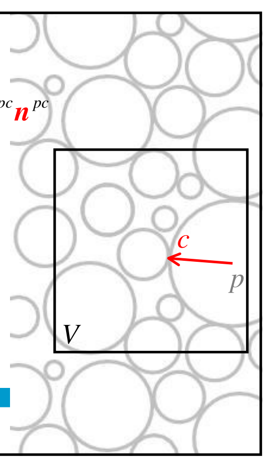
Averaging Fabric

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

Any quantity:

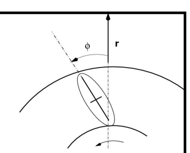
$$Q^p = \underline{\underline{\mathbf{F}}}^p = \sum_c \boldsymbol{n}^{pc}\boldsymbol{n}^{pc}$$

- Scalar: contacts
- Vector: normal
- Contact distribution



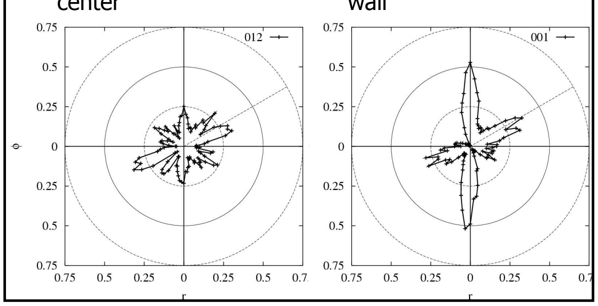
Fabric tensor

contact probability ...

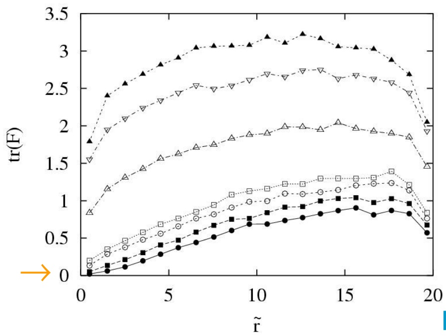


center

wall

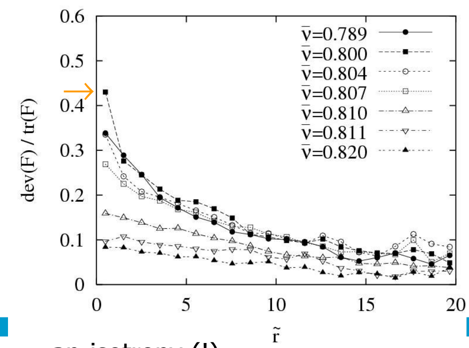


Fabric tensor (trace)



contact number density

Fabric tensor (deviator)



an-isotropy (!)

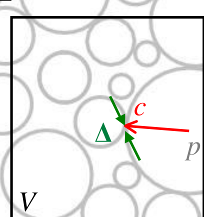
Averaging Deformations (elastic)

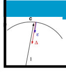
$$Q = \underline{\underline{\varepsilon}} = \frac{\pi h}{V}\left(\sum_{p \in V} w_V^p \sum_c l^{pc} \Delta^c\right) \cdot \underline{\underline{\mathbf{F}}}^{-1}$$

Deformation:

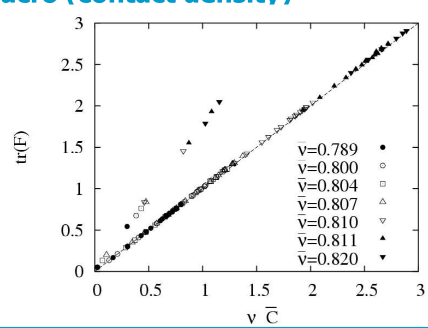
$$S = \left(\Delta^c - \underline{\underline{\varepsilon}} \cdot l^{pc}\right)^2 \quad \text{minimal !}$$

- Scalar
- Vector
- Tensor: Deformation



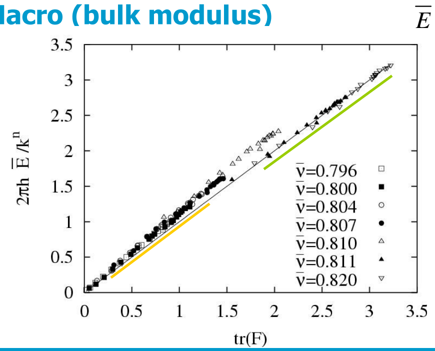


Macro (contact density)



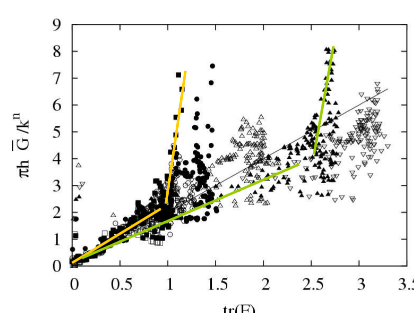
Macro (bulk modulus)

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



Macro (shear modulus)

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



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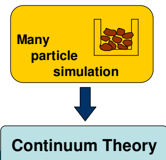


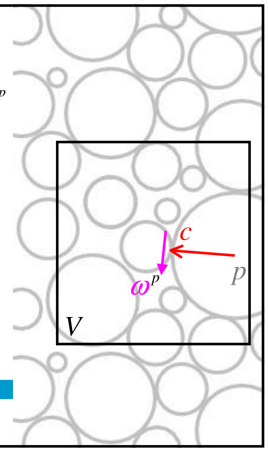
Averaging Rotations

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

Deformation:

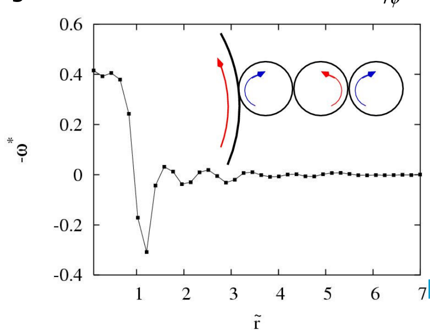
$$Q^p = \omega^p$$

- Scalar
- Vector: Spin density
- Tensor

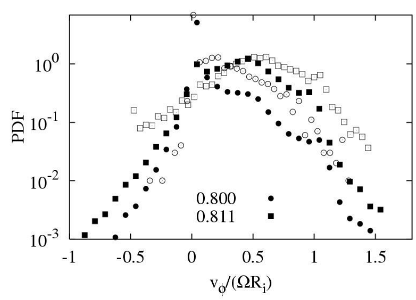


Rotations – spin density

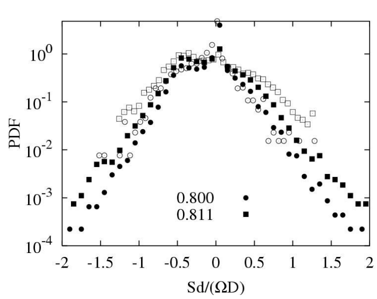
eigen-rotation: $\omega^* = \omega - W_{r\phi}$

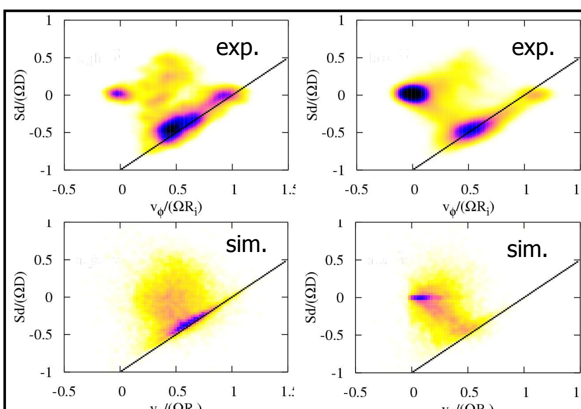


Velocity distribution



Spin distribution

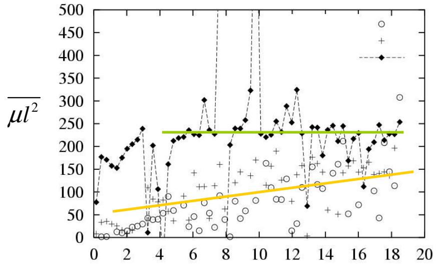




high dens. low dens.

Macro (torque stiffness)

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



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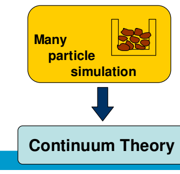
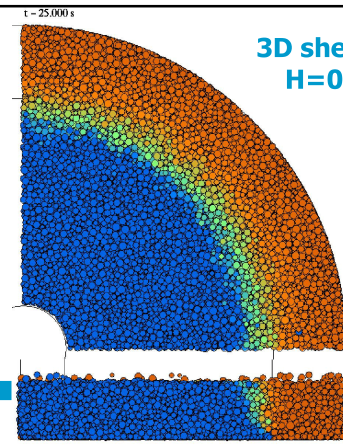
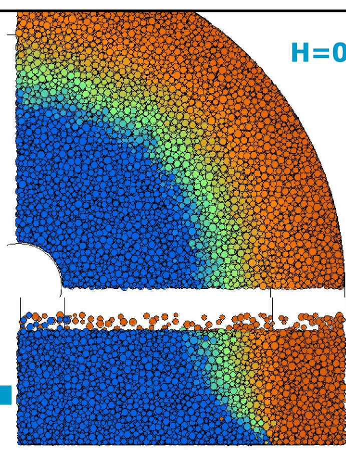


Summary

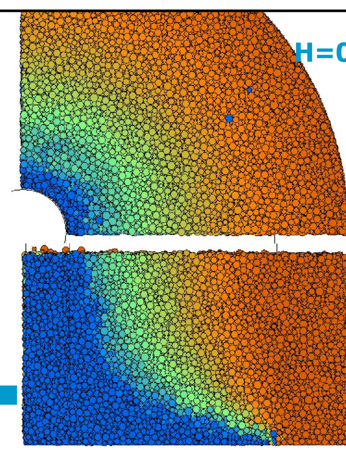
Quantitative comparison between
Experiments (2D Couette) &
MD simulations (soft disks)
Observations:
- **shear band & dilation**
- **inhomogeneous (force-chains)**
- **(almost always) an-isotropic**
- **micro-polar (rotations)**



3D shear cell H=0.016m



H=0.040m



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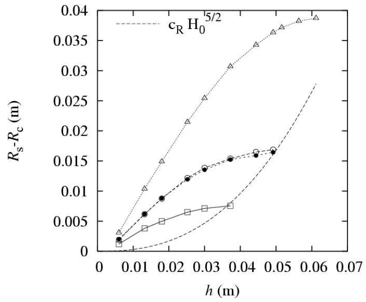
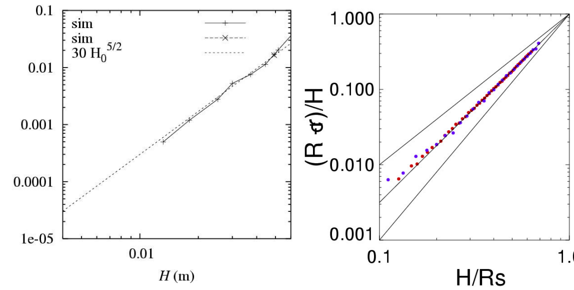
3D shear band center position



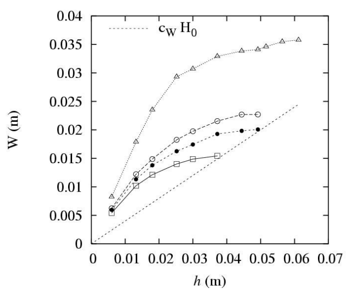
80% agreement … up to now

3D shear band center position



80% agreement … up to now

3D shear band width



80% agreement … up to now

The End