

# Particles, Granular Texture and Flow States

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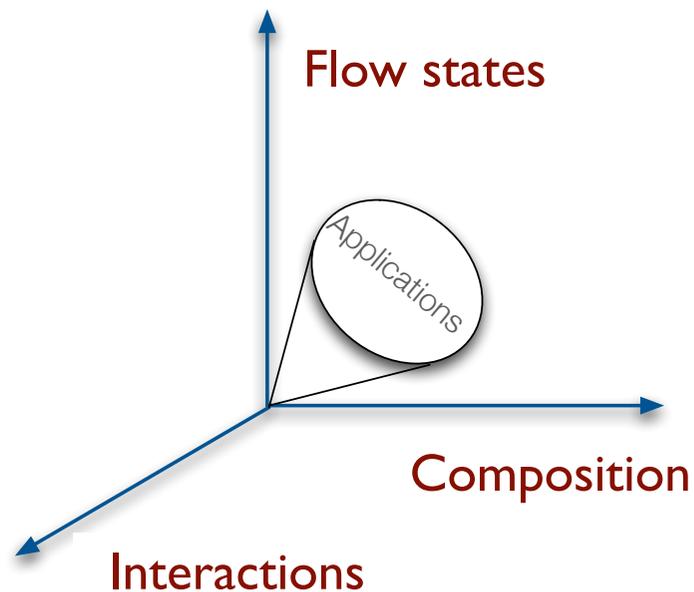
MIT, MIT Energy Initiative, Cambridge, MA, USA

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## Parameter space

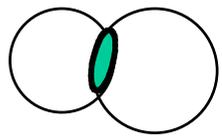
- 1) **Composition:** physical properties of particles, size distributions, shapes, particle surface, pore-filling fluids or solids
- 2) **Interactions:** friction, cohesion, couplings
- 3) **Flow states:** stress state, strain or stress rates, texture in equilibrium



## The parameter space can be reduced.

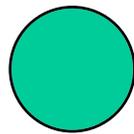
Some local parameters are ‘filtered’ by the granular microstructure and do not radiate to the macroscopic scale.

Examples: restitution coefficient and friction coefficient in quasi-static flow



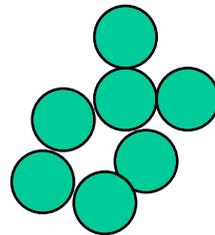
Contact

$\delta$

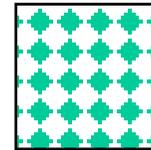


Particle

$d$

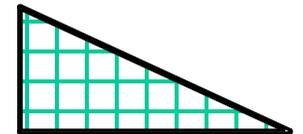


Packing



Material

RVE

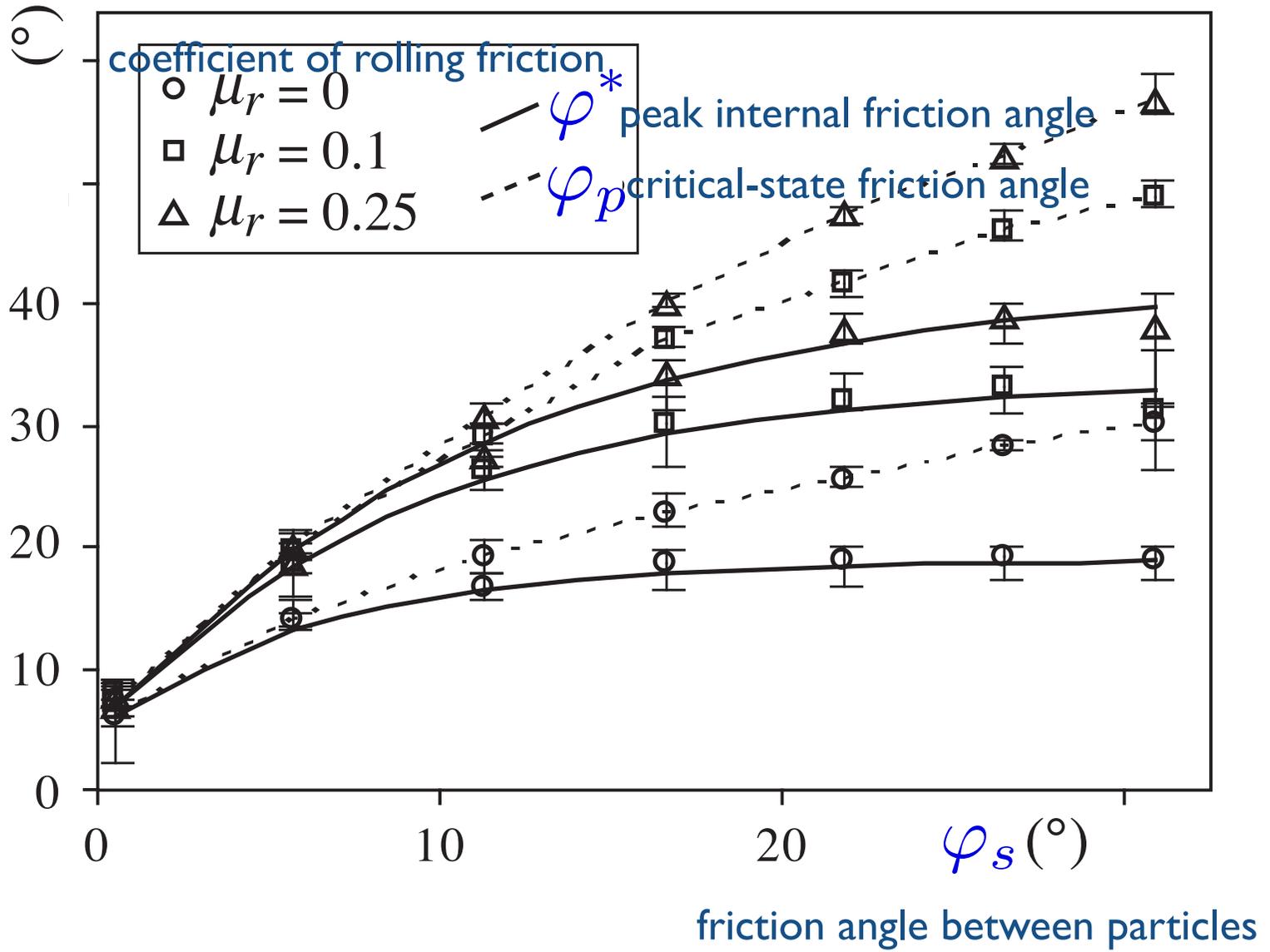


Process

BC

Scales

# quasi-static flow



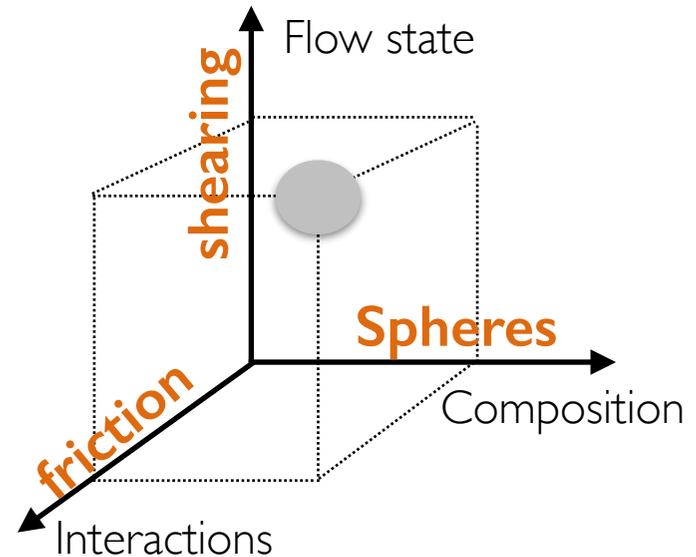
A. Taboada, N. Estrada and F. Radjai (2006), PRL 97, 098302

Some compositional parameters can be replaced by interactions (in the spirit of ‘molecular dynamics’).

DEM: 3 levels

1) **Basic** (1980s)

Spherical particles + frictional contact interactions



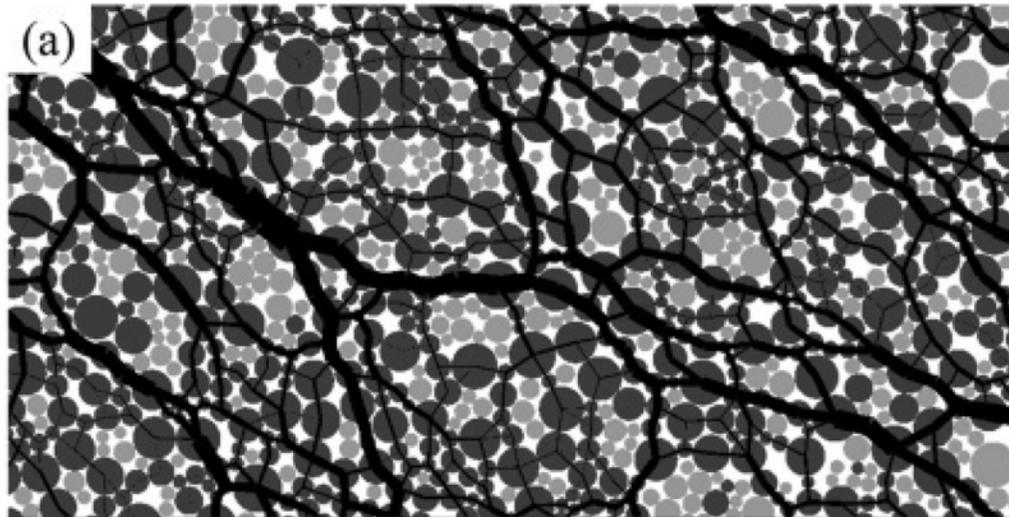
2) **Extended** (1990s)

Bonded spheres, adhesion forces (capillary, lubrication, adhesion), broad size distributions, rolling friction

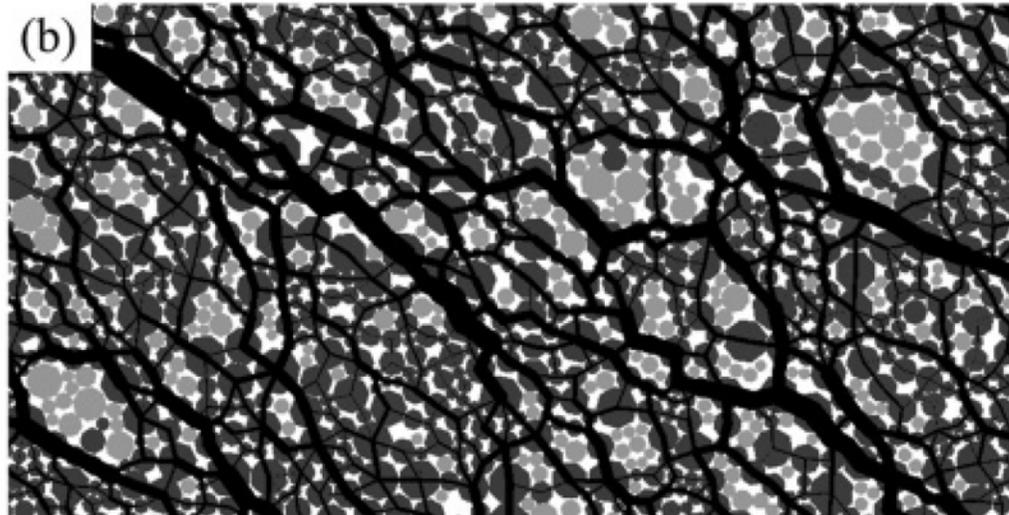
3) **Advanced** (2000s)

Aspherical particles, particle fracture, pore-filling phases (liquid, solid)

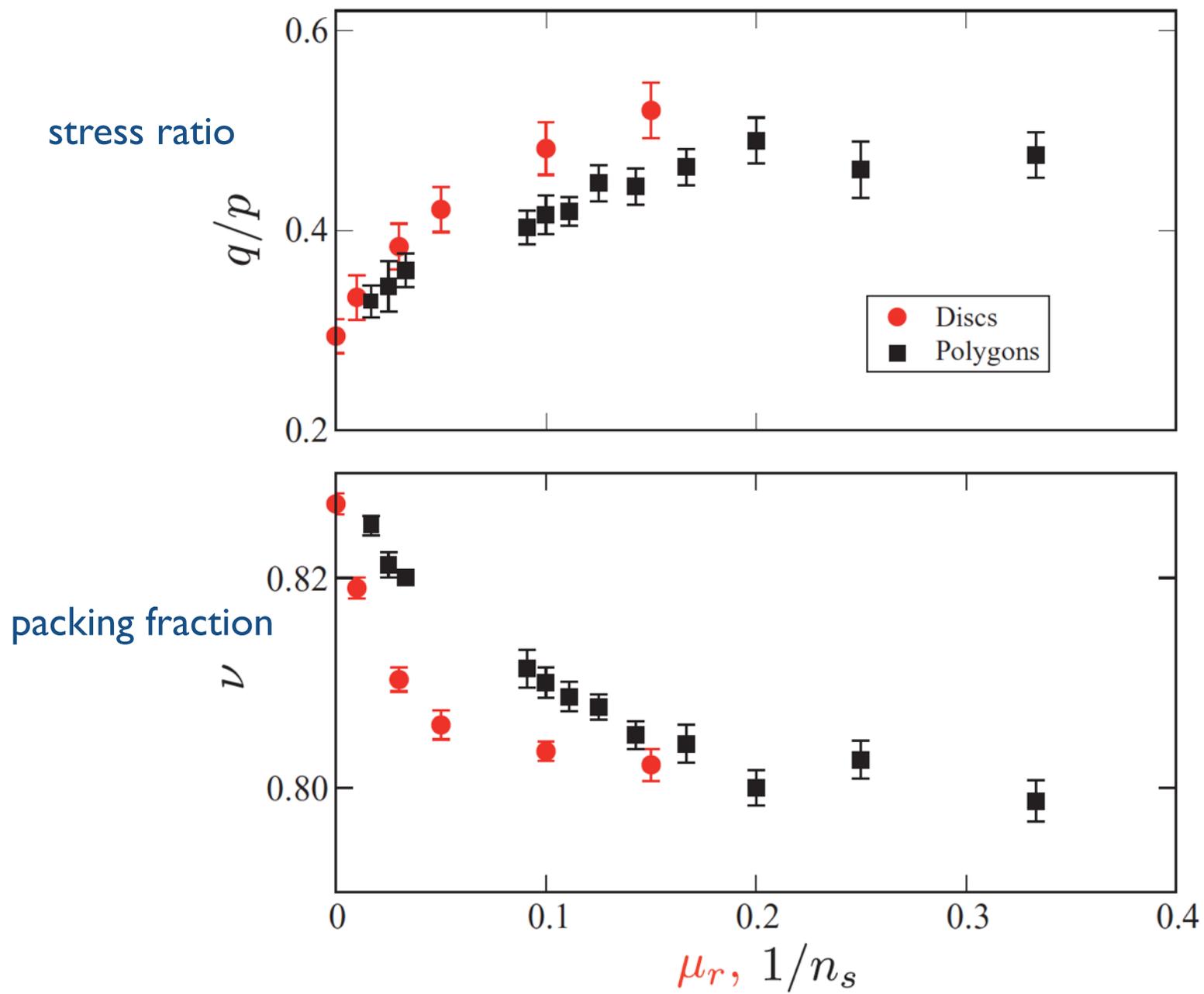
# Example: Particle shape vs. rolling resistance

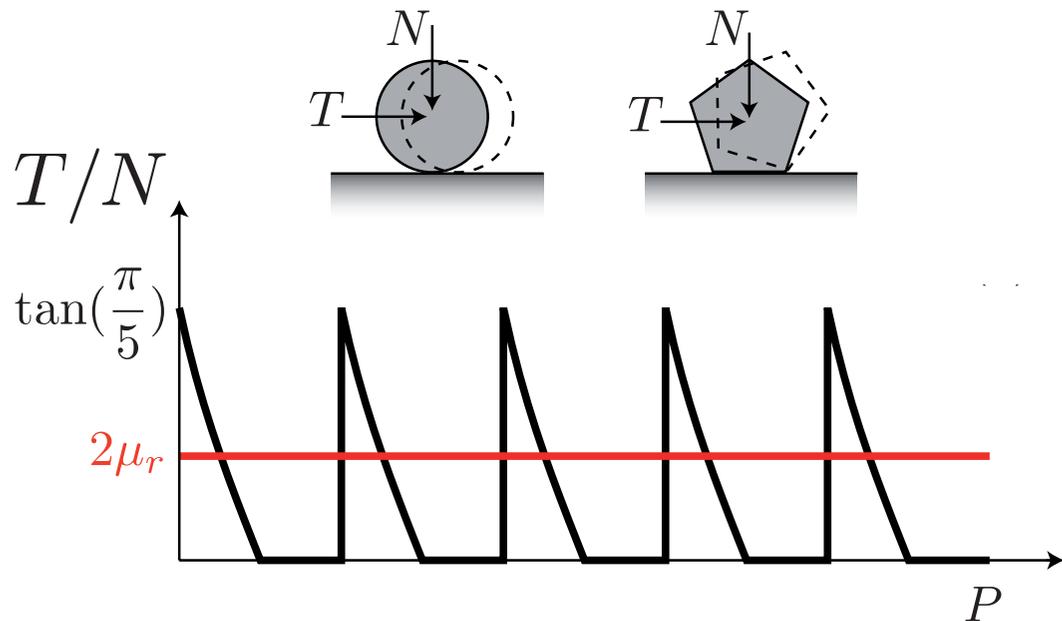


disk  
 $\mu_r$   
rolling friction coefficient



polygons  
 $n_s$   
number of sides





Energy dissipation per cycle:

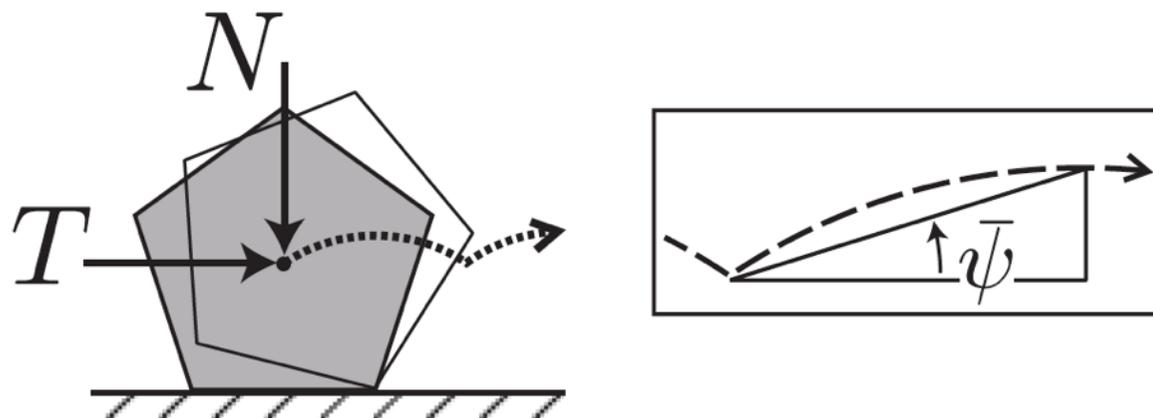
polygon

$$W_p = n_s(1 - \cos(\pi/n_s))R_p N$$

disk

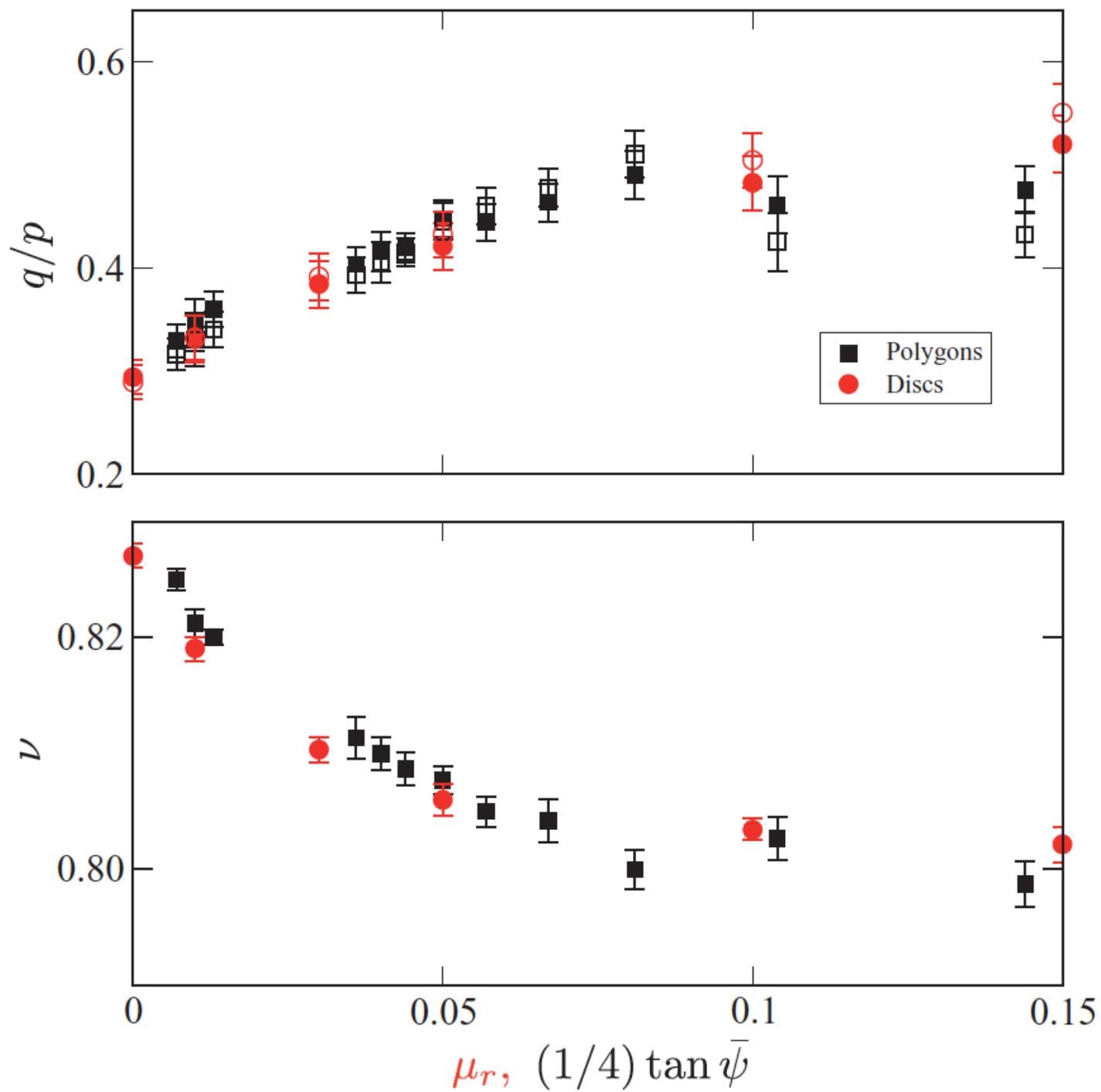
$$W_d = 4\pi \mu_r R_d N$$

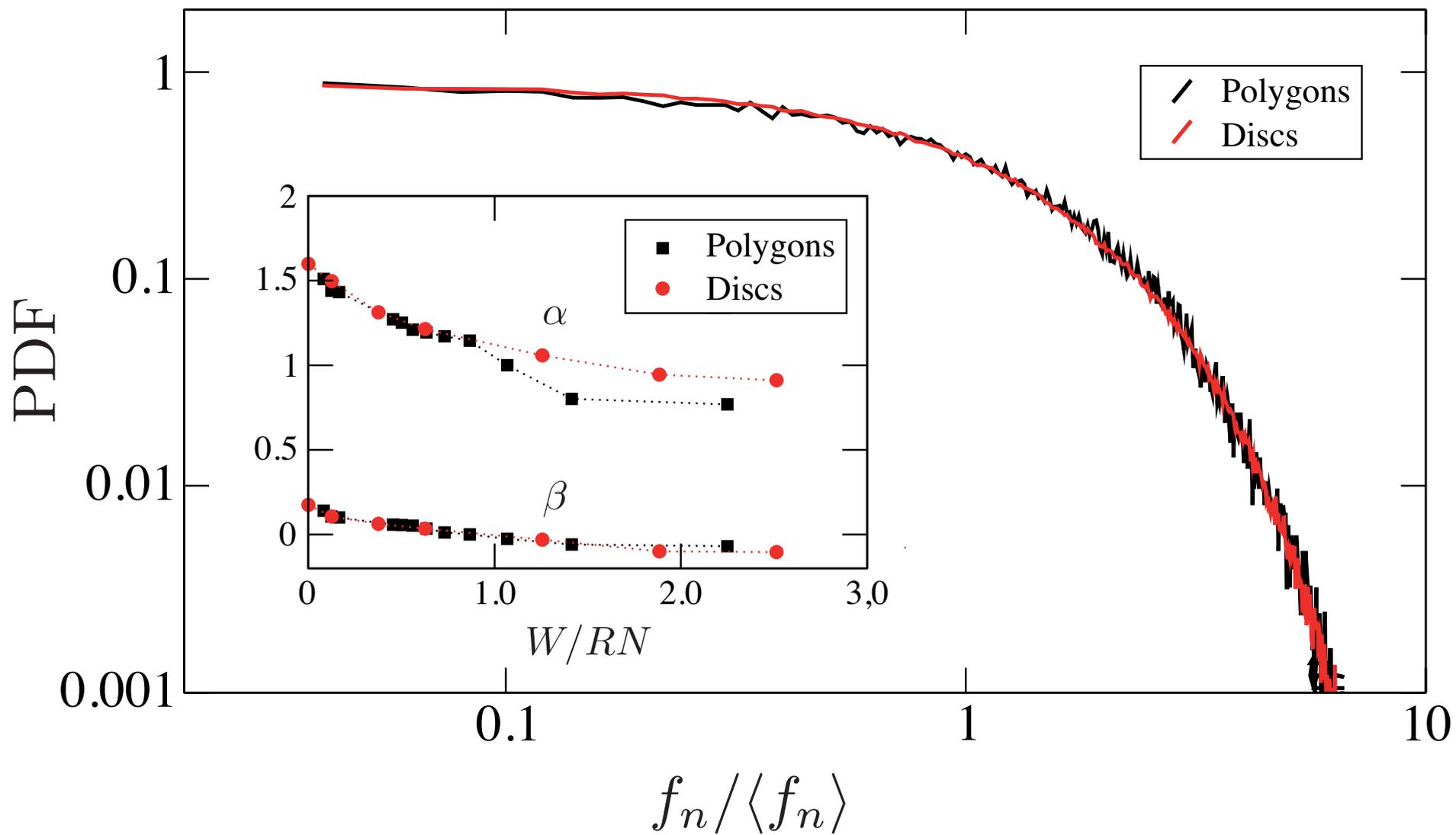
$$W_p = W_d \Rightarrow$$



$$\mu_r = (1/4) \tan \bar{\psi}$$

local dilatancy angle





Dimensionless parameters can be combined: look for combinations that lead to equivalent macroscopic behaviors (in terms of shear strength and packing fraction).

## Example: immersed granular flows

Flow-wise periodic BC

Homogeneous shearing of fluid

Confining pressure on grains

Parameters:

$$\eta_f \in [\eta_w, 1000\eta_w]$$

fluid viscosity

$$\dot{\gamma} \in [0.5, 5.5] \text{ s}^{-1}$$

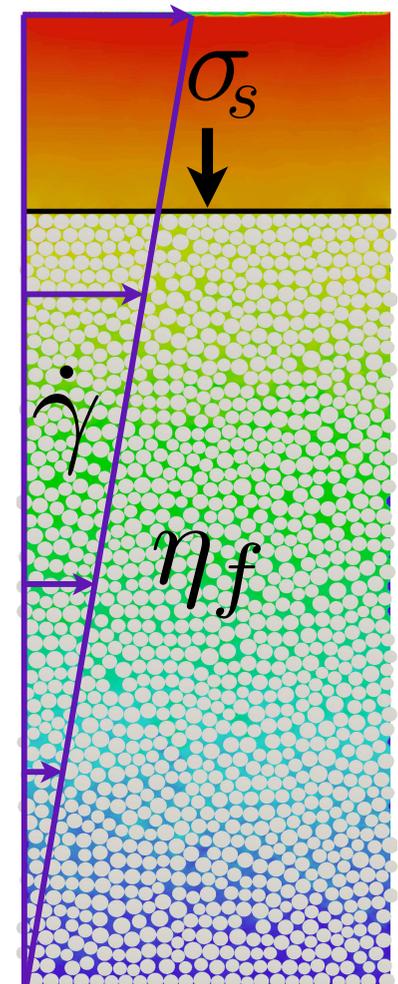
shear rate

$$\sigma_s \in [20, 120] \text{ Pa}$$

confining stress

$$\rho_s/\rho_f \in \{0.5, 1.2, 2.6, 4\}$$

relative solid/fluid density



# Numerical simulations

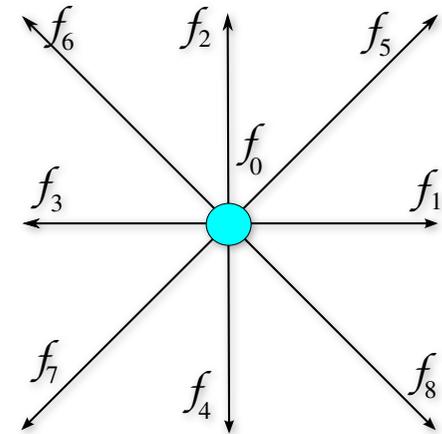
Discrete Element Method (**DEM**) + Lattice Boltzmann Method (**LBM**)

## LBM

$$f_i(\vec{r} + \Delta t \vec{e}_i, t + \Delta t) - f_i(\vec{r}, t) = \Omega_i$$

$$\Omega_i = -\frac{1}{\tau} (f_i(\mathbf{r}, t) - f_i^{eq}(\mathbf{r}, t)), \quad i \in \{0, 1, \dots, 8\}$$

BGK collision operator

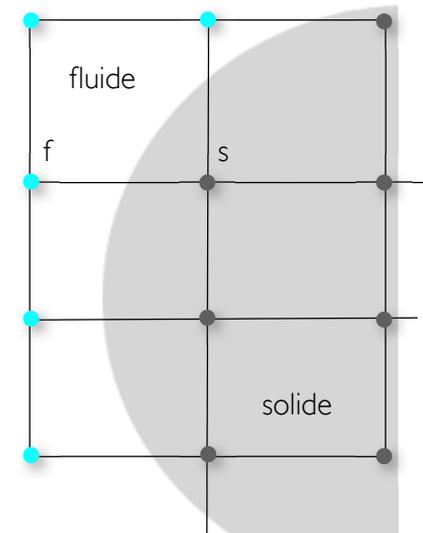


## DEM

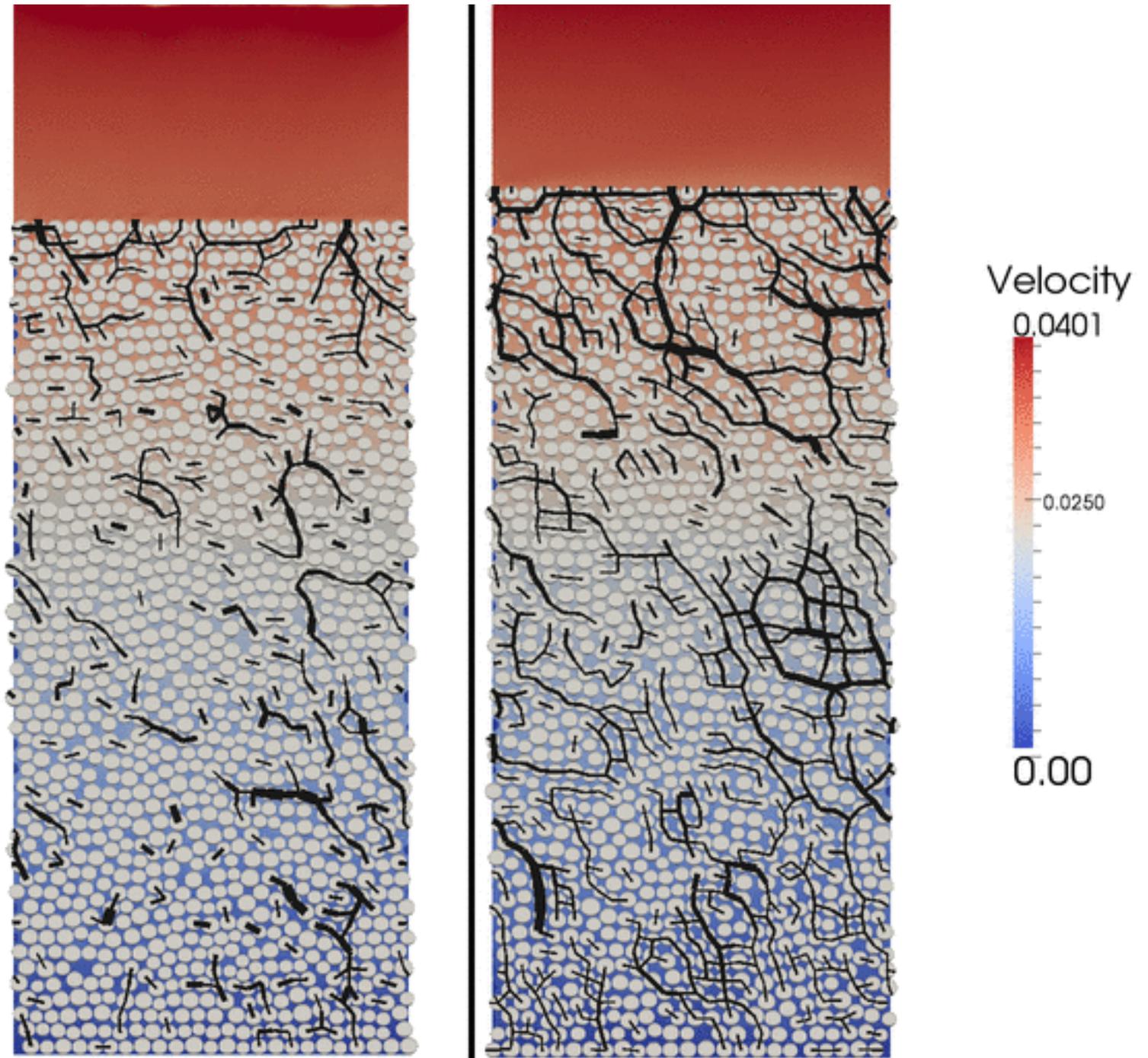
$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i, \quad i = 1 \dots N$$

$$\mathbf{F}_i = \sum_{j \neq i} \mathbf{F}_{c_{ij}} + \mathbf{F}_{g_i} + \mathbf{F}_{h_i}$$

2DQ9



Interface

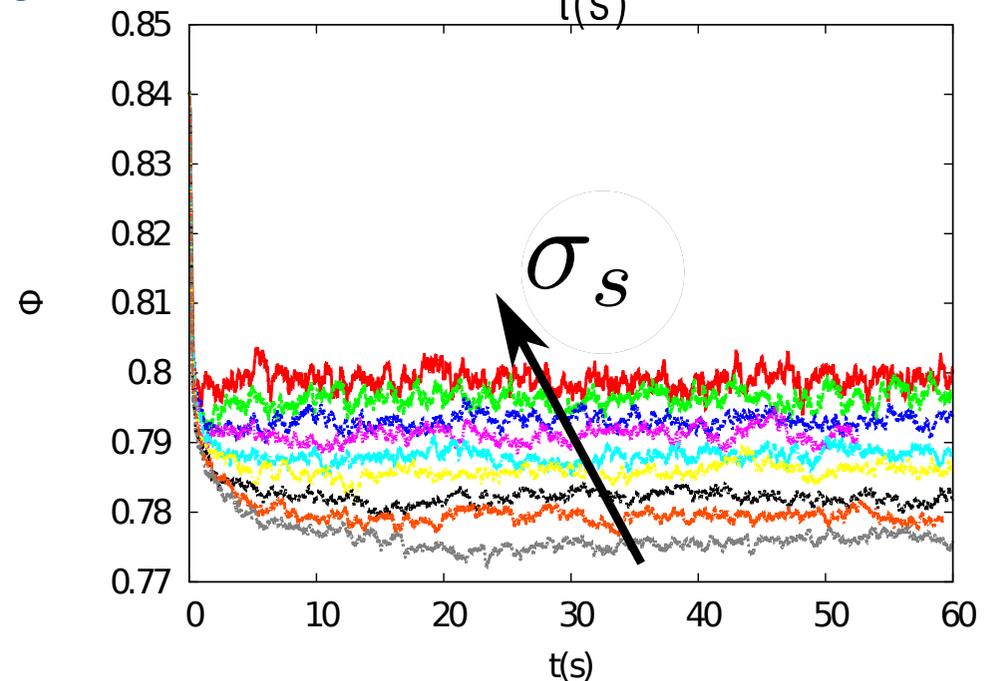
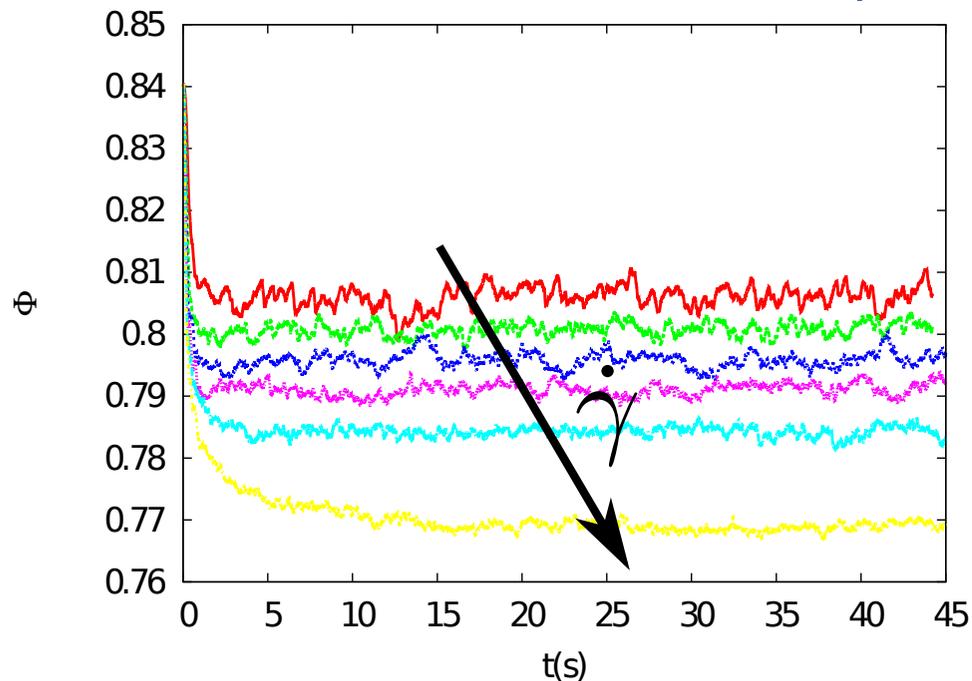
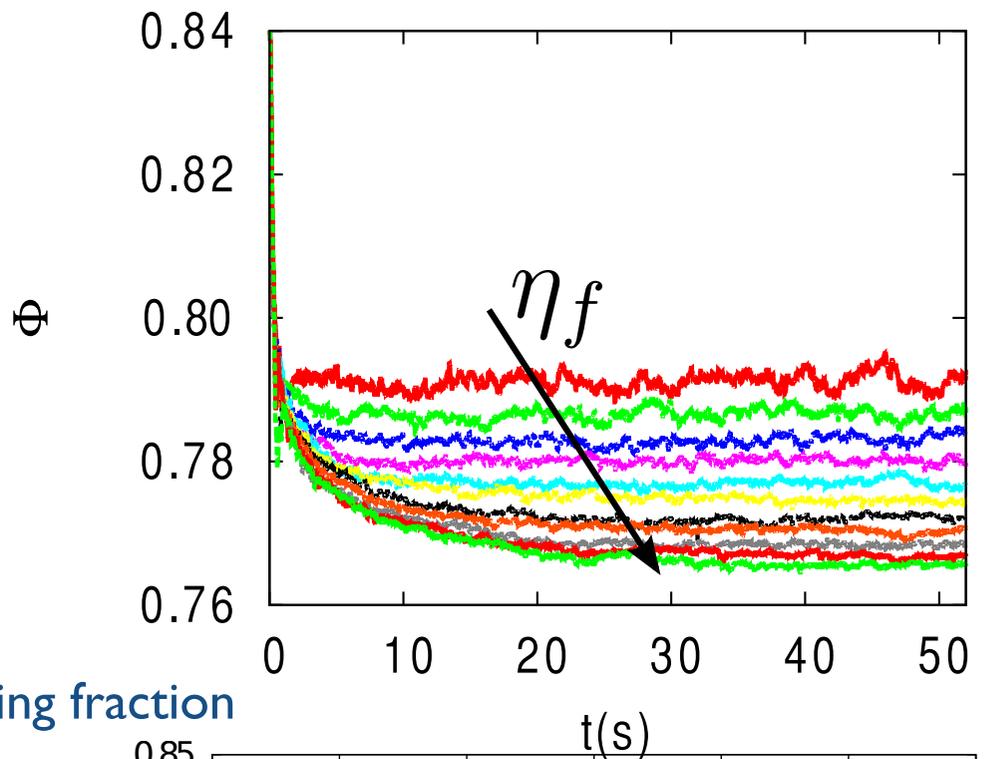


Steady flow: mean values and their temporal variability measured during the steady state

70 Number of simulations

$10^5$  CPU hours

30 To Data



## times and force scales

We separate the time scales associated with confining pressure and drag force:

$$t^2 = \frac{md}{F} \quad \text{Dimensional relation}$$

$F_s = \sigma_s d$	Static force	$\Rightarrow$	$t_s = d \left( \frac{\rho_s}{\sigma_s} \right)^{\frac{1}{2}}$
$F_v = \eta_f \dot{\gamma} d$	Drag force	$\Rightarrow$	$t_v = d \left( \frac{\rho_s}{\eta_f \dot{\gamma}} \right)^{\frac{1}{2}}$
$F_i = \rho_s (d \dot{\gamma})^2 d$	Inertial force	$\Rightarrow$	$t_i = \dot{\gamma}^{-1}$

$$\frac{t_e}{t_i} = \left( \frac{t_s}{t_v} \right)^2$$

$$t_e = \frac{\eta_f}{\sigma_s}$$

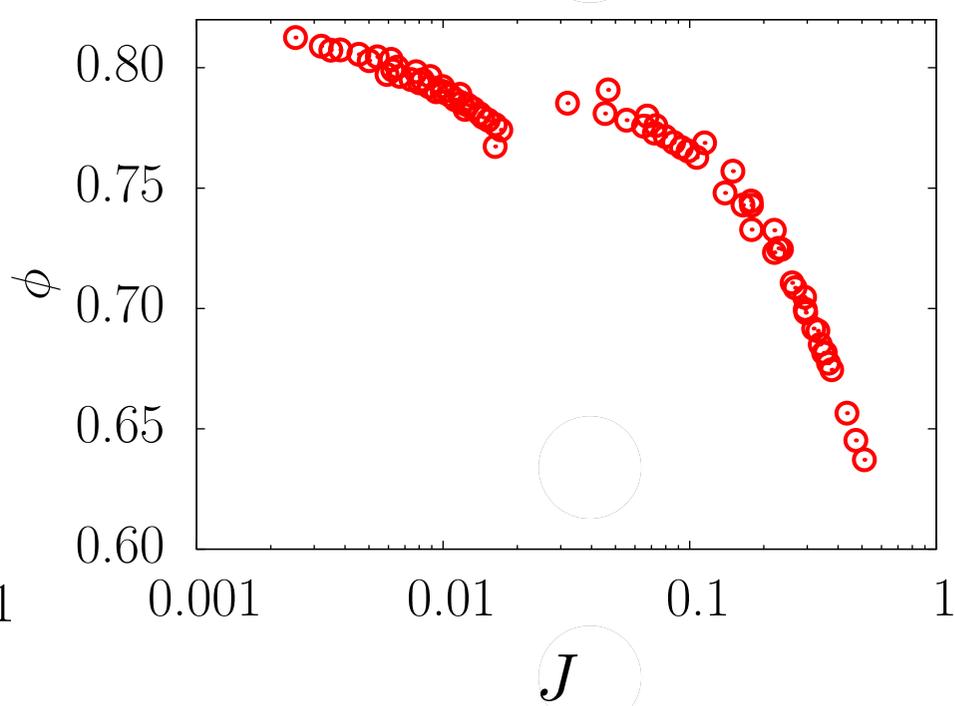
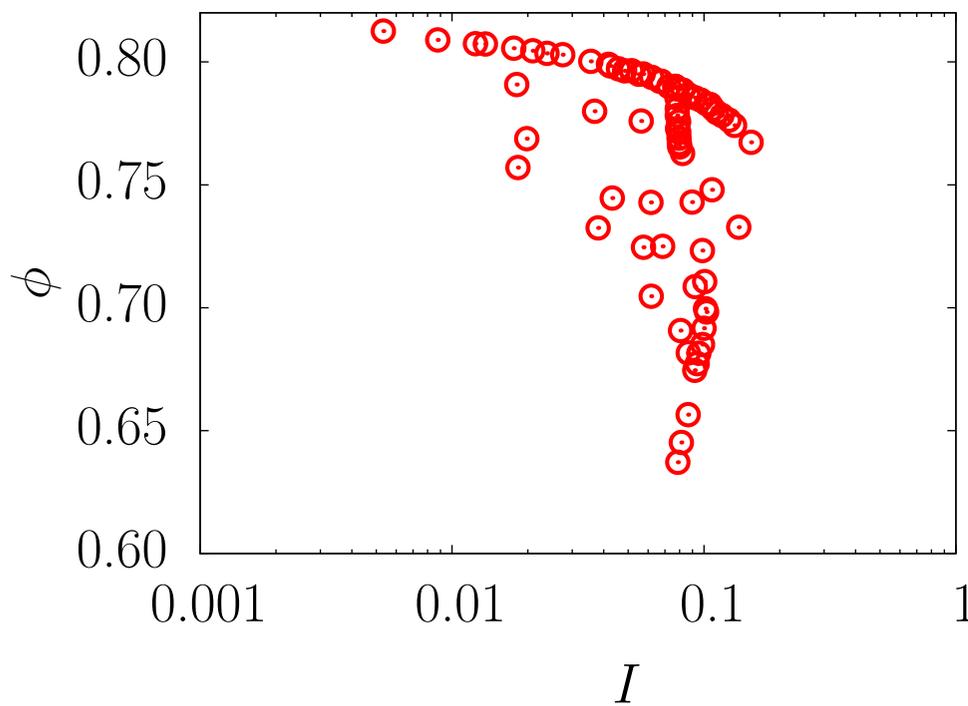
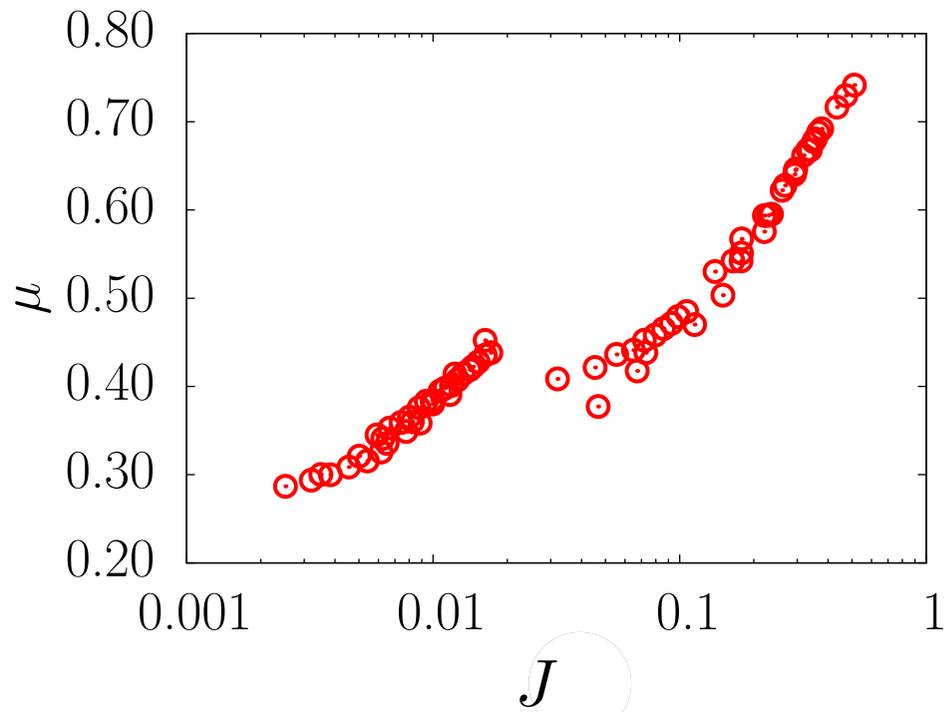
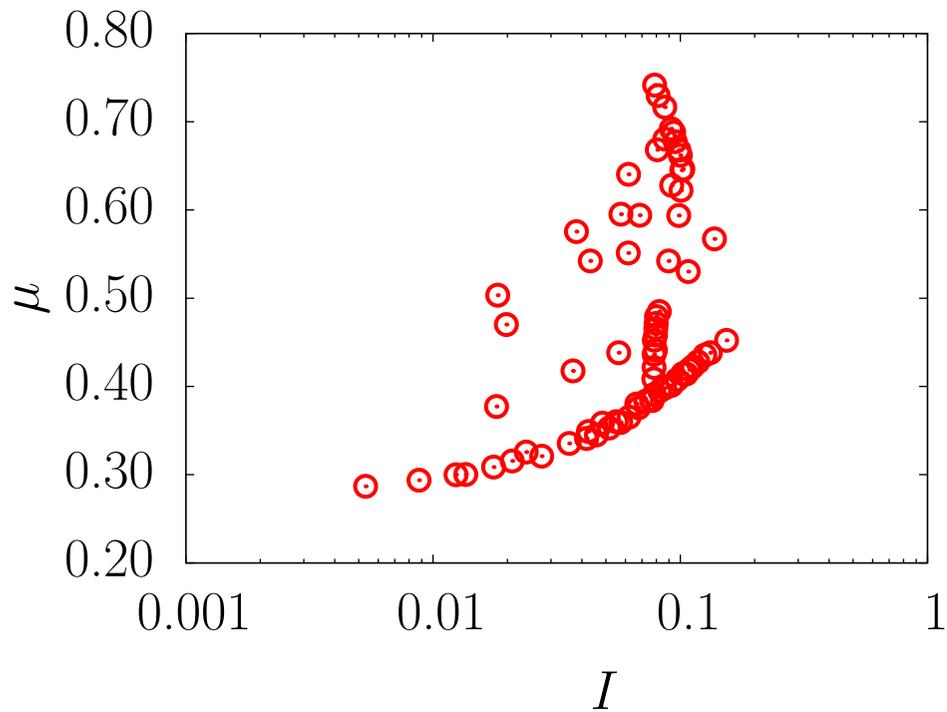
$$I = \frac{t_s}{t_i} = \left( \frac{\sigma_i}{\sigma_s} \right)^{\frac{1}{2}} = \dot{\gamma} d \left( \frac{\rho_s}{\sigma_s} \right)^{\frac{1}{2}}$$

$$J = \frac{t_s}{t_v} = \left( \frac{\sigma_v}{\sigma_s} \right)^{\frac{1}{2}} = \left( \frac{\eta_f \dot{\gamma}}{\sigma_s} \right)^{\frac{1}{2}}$$

$$St = \left( \frac{t_v}{t_i} \right)^2 = \frac{\sigma_i}{\sigma_v} = \frac{I^2}{J^2} = \frac{\rho_s d^2 \dot{\gamma}}{\eta_f}$$

Stokes number

Can the rheology be described as a function of a **single dimensionless parameter** combining the above numbers? Such a description should **include both inertial dry granular flows and dense non-brownian suspensions.**



# Unified rheology

$$\tau_c = \mu_c \sigma_s \quad \text{Static stress}$$

$$\tau_v = k_v \eta_f \dot{\gamma} \quad \text{Viscous stress}$$

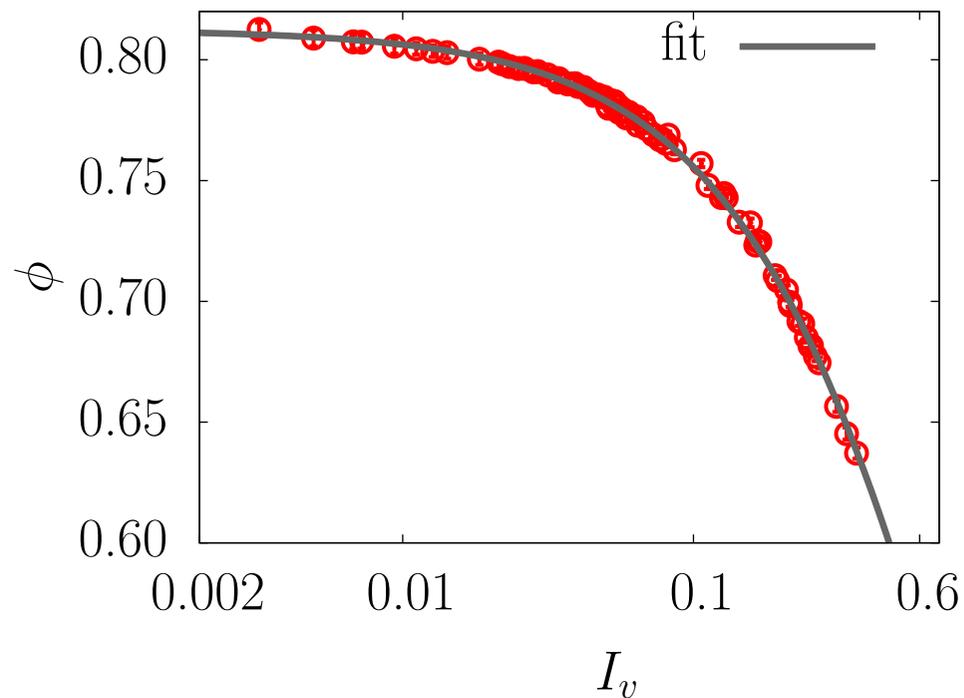
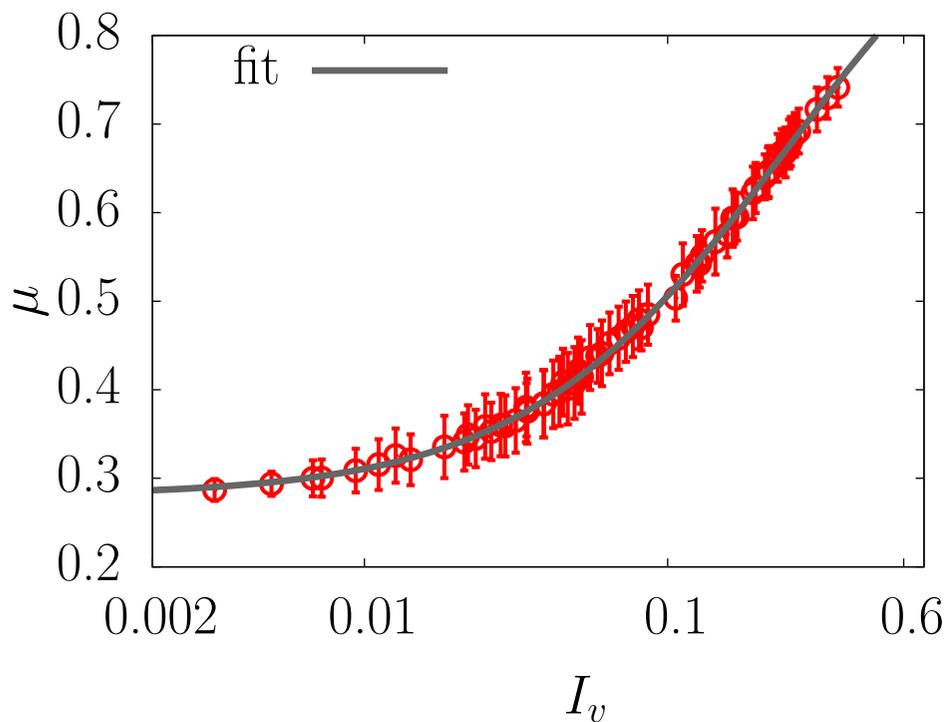
$$\tau_i = k_i \rho_s (d\dot{\gamma})^2 \quad \text{Inertial stress}$$

$\tau - \tau_c$  is expected to be a function of  $\tau_v + \tau_i$

$$I_v^2 = \frac{\rho_s (d\dot{\gamma})^2 + \alpha_v \eta_f \dot{\gamma}}{\sigma_s} = (I^2 + \alpha_v J^2) = I^2 \left(1 + \frac{\alpha_v}{St}\right)$$

$$\Rightarrow I_v = I(1 + \alpha_v/St)^{1/2}$$

modified inertial number or **Visco-inertial number**



$$\alpha_v = 2$$

$$\mu = \mu_c + \frac{\mu_{max} - \mu_c}{1 + I_{v0}/I_v}$$

$$\phi(I_v) = \frac{\phi_c}{1 + aI_v}$$

$$\mu_c = 0.280 \pm 0.002$$

$$\phi_c = 0.8124 \pm 0.0003$$

$$I_{v0} \simeq 0.246 \pm 0.008$$

$$a = 0.750 \pm 0.003$$

$$\mu_{max} = 1.063 \pm 0.0124$$

Viscous description at imposed packing fraction:

$$\tau = \eta_t \dot{\gamma} = c_t \sigma_s I_v^2$$

$$\sigma_n = \eta_n \dot{\gamma} = c_n \sigma_s I_v^2$$

$\eta_t$  and  $\eta_n$  shear and normal effective viscosities

$\sigma_s = \sigma_n$  stress imposed on the granular phase only

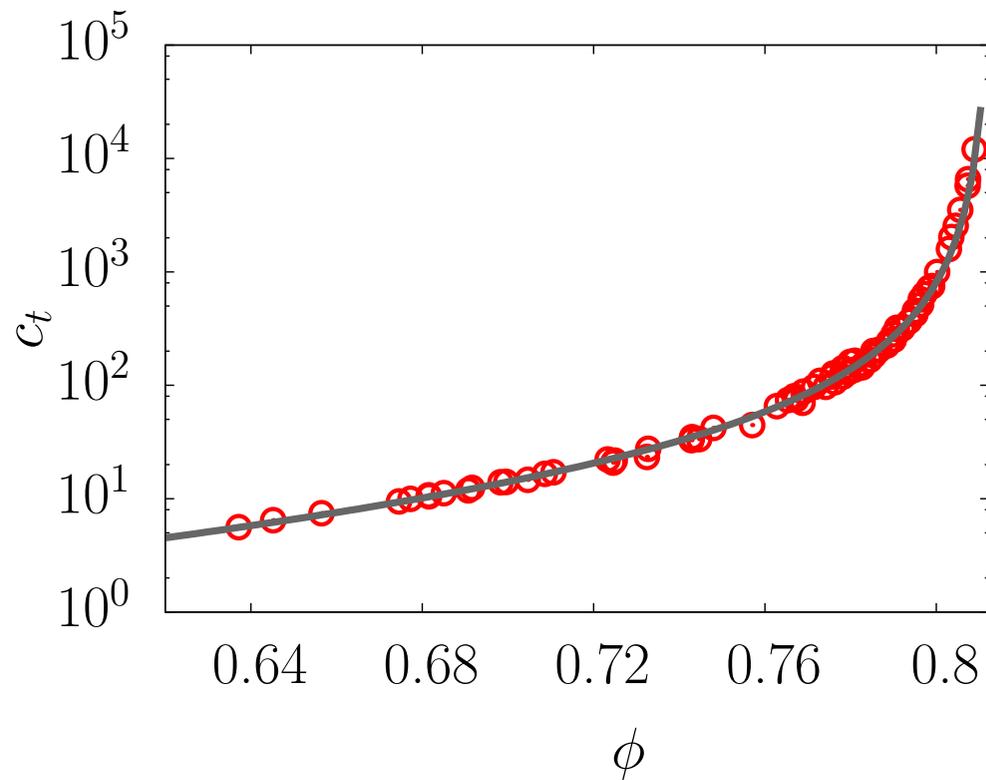
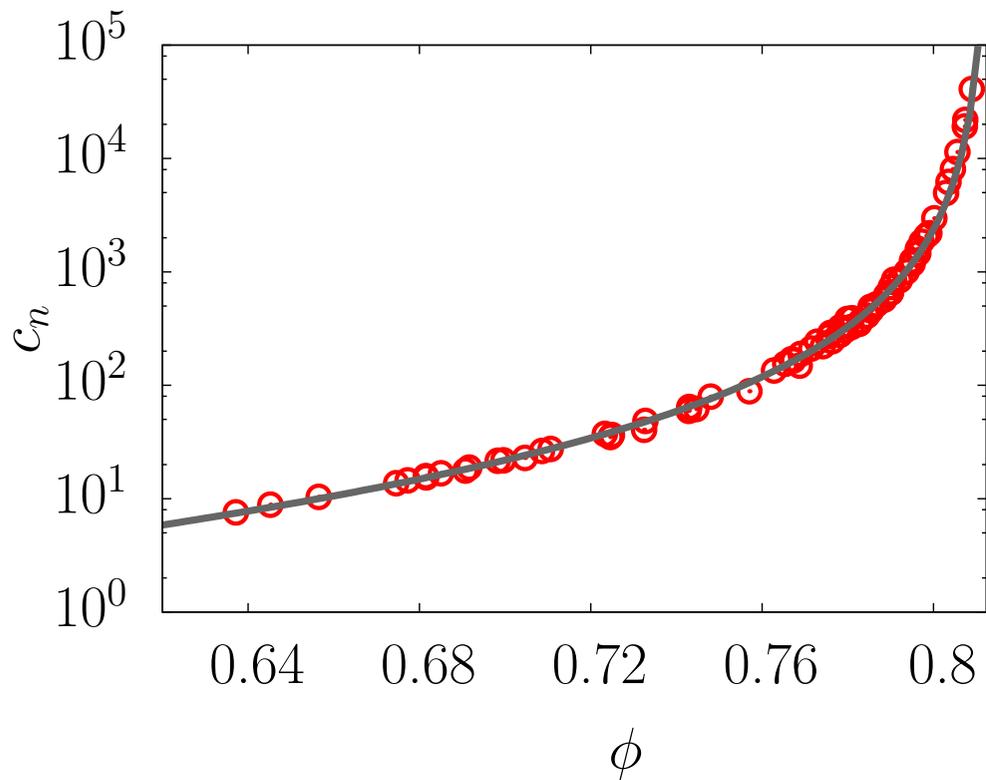
⇒

$$c_n = \frac{1}{I_v^2} \quad c_t = \frac{\mu}{I_v^2}$$

normal

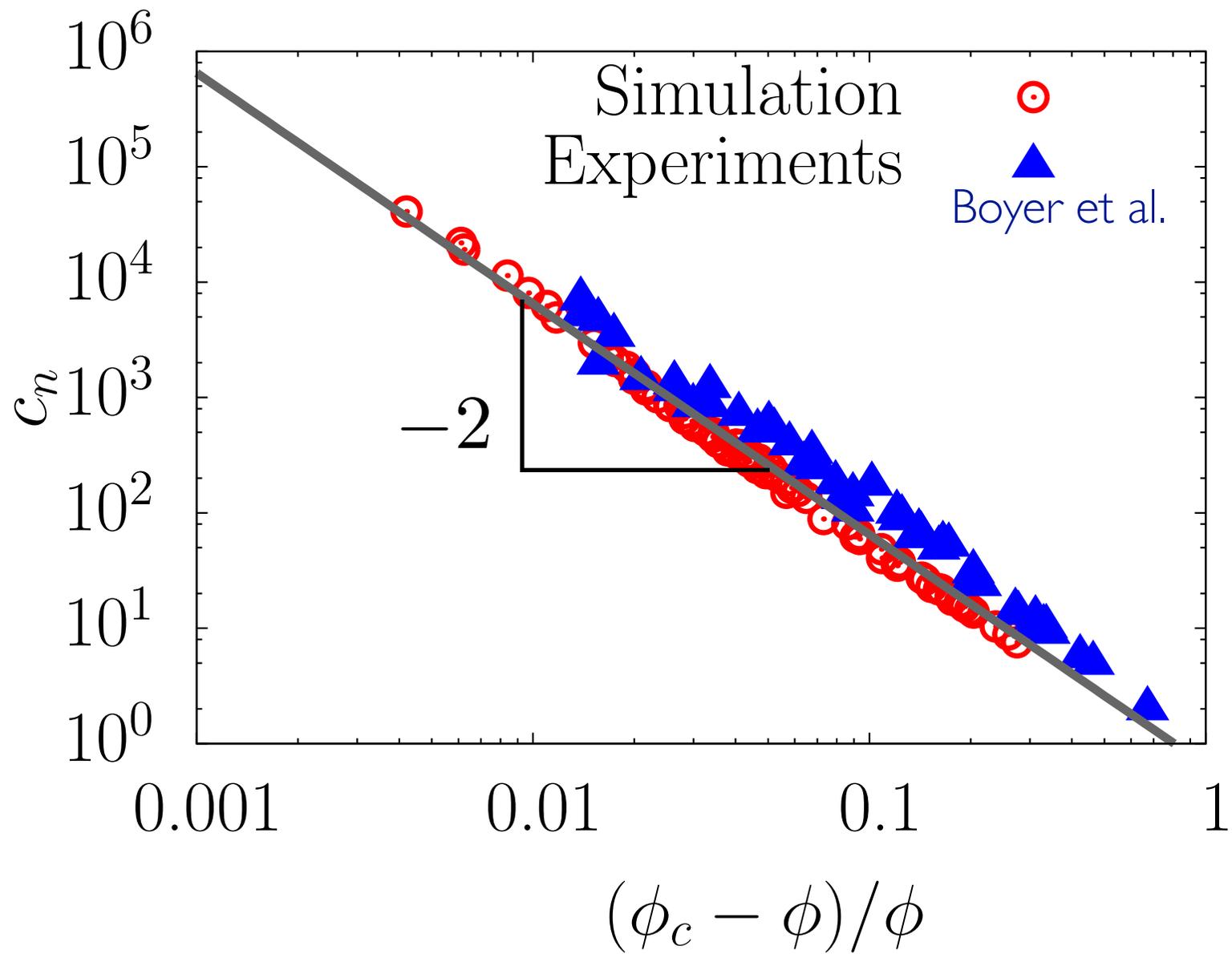
shear

effective viscosity effective viscosity



$$c_n \simeq a^2 \left( \frac{\phi}{\phi_c - \phi} \right)^2$$

$$c_t \simeq a^2 \left( \frac{\phi}{\phi_c - \phi} \right)^2 \left\{ \mu_c + \frac{\mu_{max} - \mu_c}{1 + aI_{v0} \frac{\phi}{\phi_c - \phi}} \right\}$$





The DEM is a powerful tool when combined with a proper texture analysis

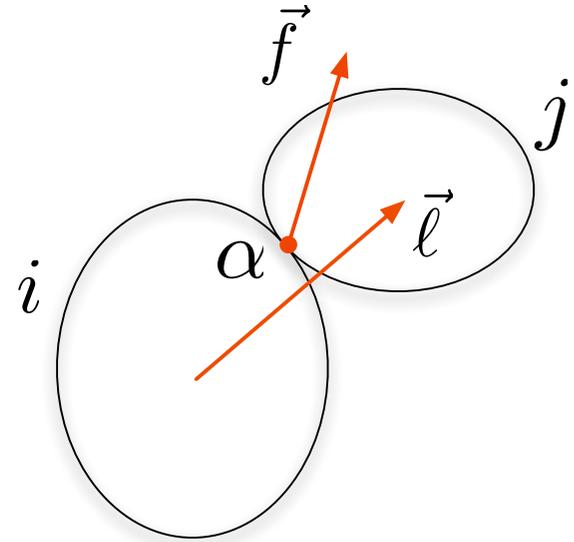
The microstructure is closely related to the stress state.

$$\sigma_{ij} = n_b \langle \ell_i^\alpha f_j^\alpha \rangle_\alpha$$

$n_b$  number density of contacts

$\vec{f}^\alpha$  contact force

$\vec{\ell}^\alpha$  branch vector



For the stress tensor to be a **state function**, the internal state must be represented by the discrete set:

$$\{\vec{f}^\alpha, \vec{\ell}^\alpha\}$$

$$\Rightarrow \sigma_{ij} = n_b \int_{\mathcal{A}_\ell} \int_{\mathcal{A}_f} \ell_i f_j P_{\ell f}(\vec{\ell}, \vec{f}) d\vec{\ell} d\vec{f}$$

$$\vec{f} = f_n \vec{n} + f_t \vec{t} \quad \vec{\ell} = \ell_n \vec{n} + \ell_t \vec{t}$$

$$p = \frac{n_c}{2} (\sigma_1 + \sigma_2) = \frac{n_c}{2} \langle f_n \ell_n + f_t \ell_t \rangle$$

2D

$$q = \frac{n_c}{2} (\sigma_1 - \sigma_2) = \frac{n_c}{2} \langle (f_n \ell_n + f_t \ell_t) \cos 2\theta + (f_n \ell_t + f_t \ell_n) \sin 2\theta \rangle$$

## Harmonic approximation

$$2\text{D: } \vec{n} = (\cos \theta, \sin \theta)$$

$$P(\theta) \simeq \frac{1}{2\pi} \{1 + a_b \cos 2(\theta - \theta_b)\}$$

$$\langle \ell \rangle(\theta) \simeq \ell_m \{1 + a_\ell \cos 2(\theta - \theta_b)\}$$

$$\langle f_n \rangle(\theta) \simeq f_m \{1 + a_n \cos 2(\theta - \theta_f)\}$$

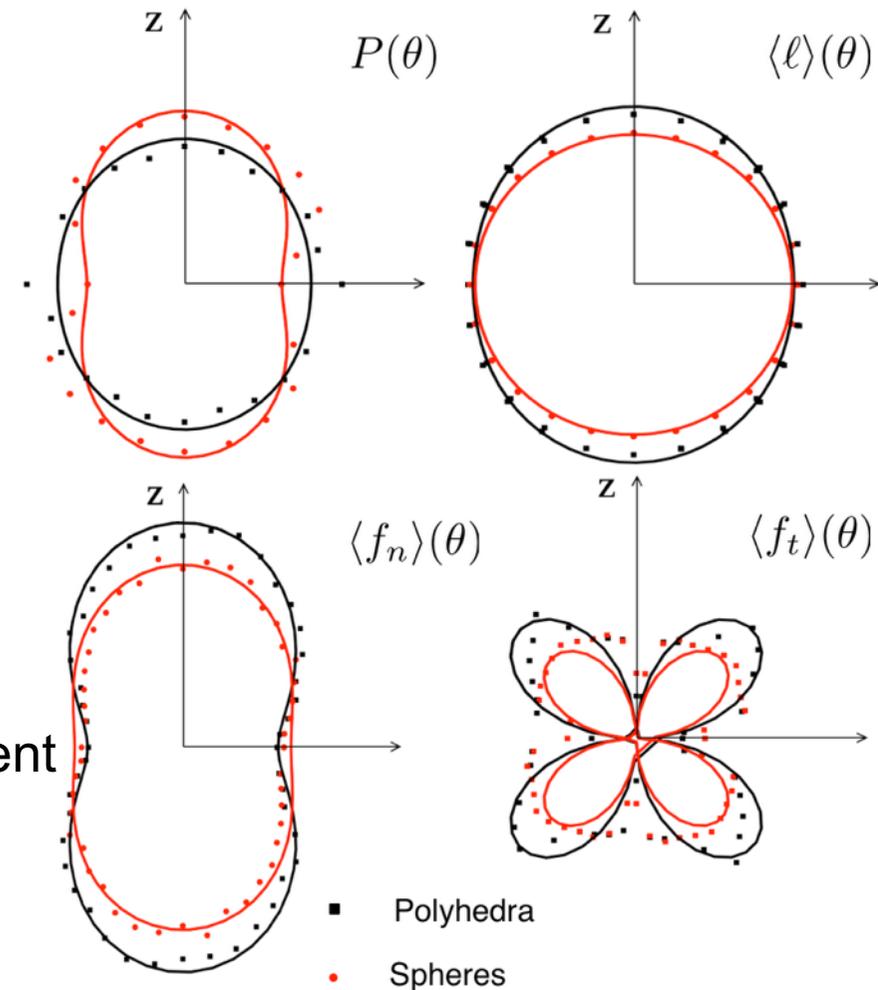
$$\langle f_t \rangle(\theta) \simeq f_m a_t \sin 2(\theta - \theta_f)$$

The last relation is imposed by the requirement of the balance of force moments:

$$\int P(\theta) \langle f_t \rangle(\theta) d\theta = 0$$

State parameters:

$$\mathcal{F} = \{z, a_b, a_\ell, a_n, a_t\}$$



E. Azéma, F. Radjai, G. Saussine, *Mech. Mat.* 41, 2009

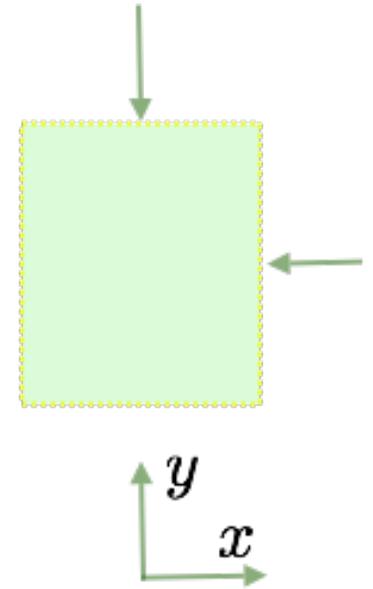
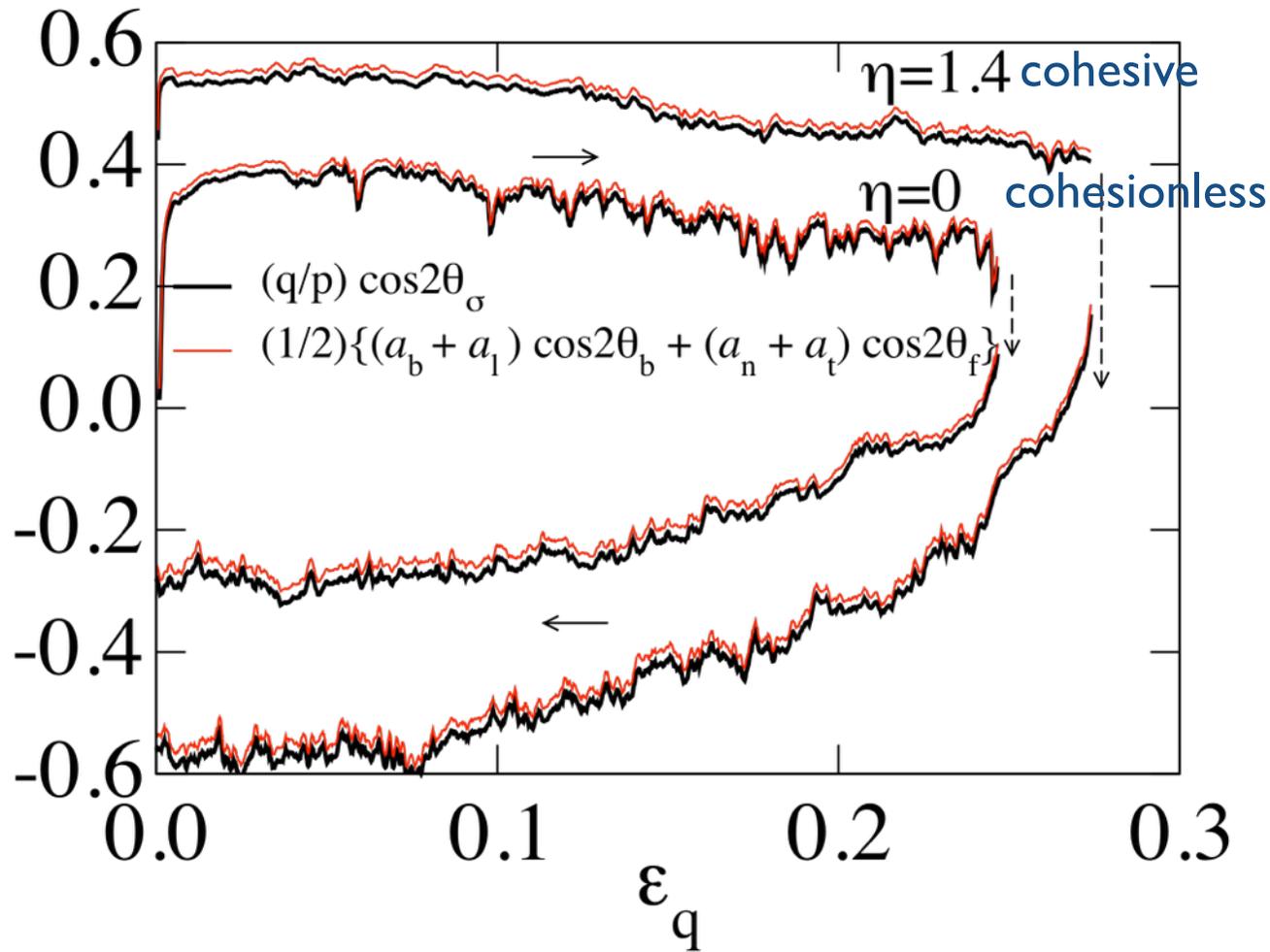
⇒ Within the harmonic representation of fabric and force states, and keeping only the linear terms in anisotropies, the expression of the stress tensor leads to two equations:

$$p \simeq \frac{1}{2} n_b \ell_m f_m$$

$$\frac{q}{p} \cos 2\theta_\sigma \simeq \frac{1}{2} \{ (a_b + a_\ell) \cos 2\theta_b + (a_n + a_t) \cos 2\theta_f \}$$

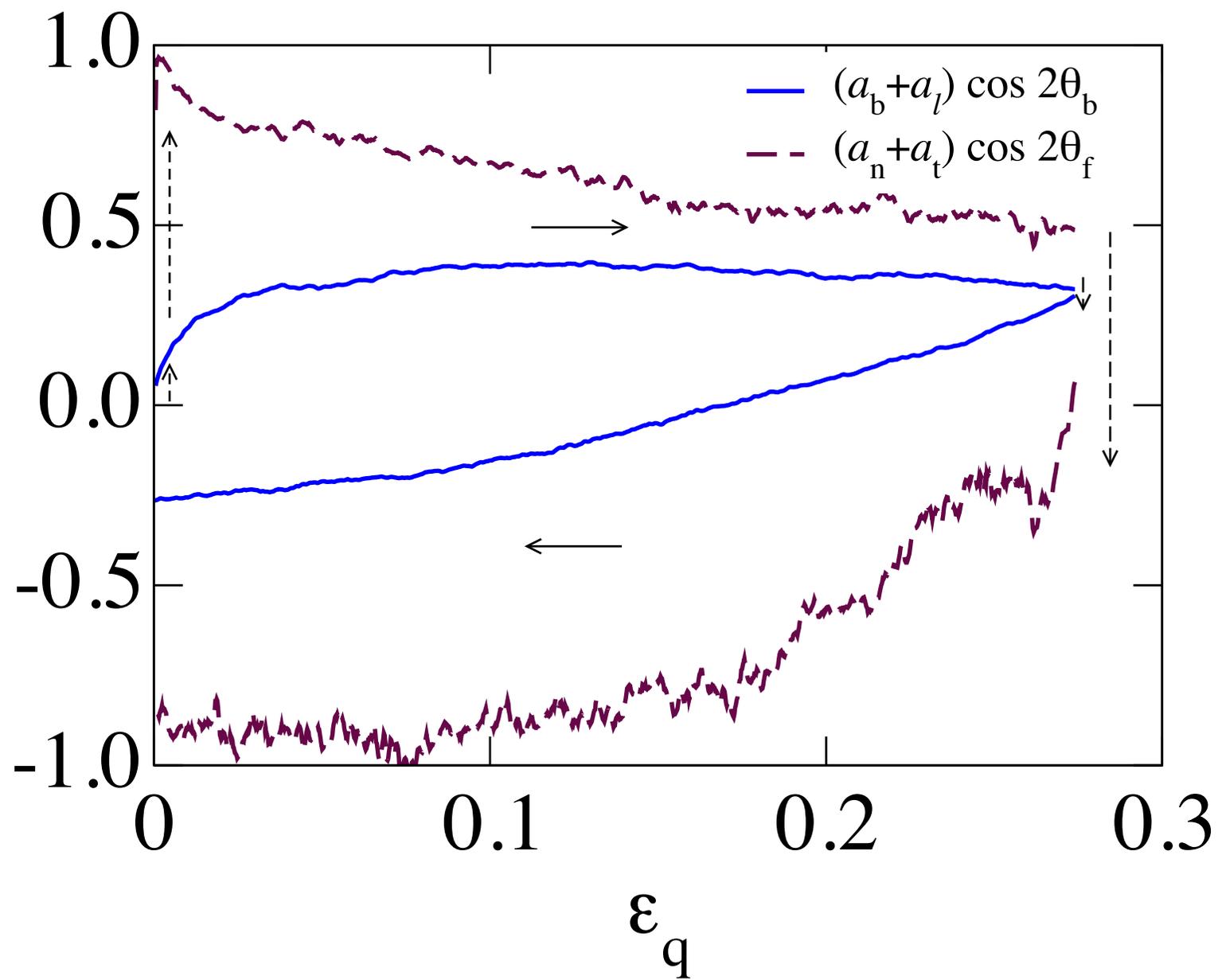
The first equation is the static analog of the **ideal gas** law for kinetic pressure. The second equation states that the stress deviator is fully dependent on the force and fabric anisotropies and their privileged directions.

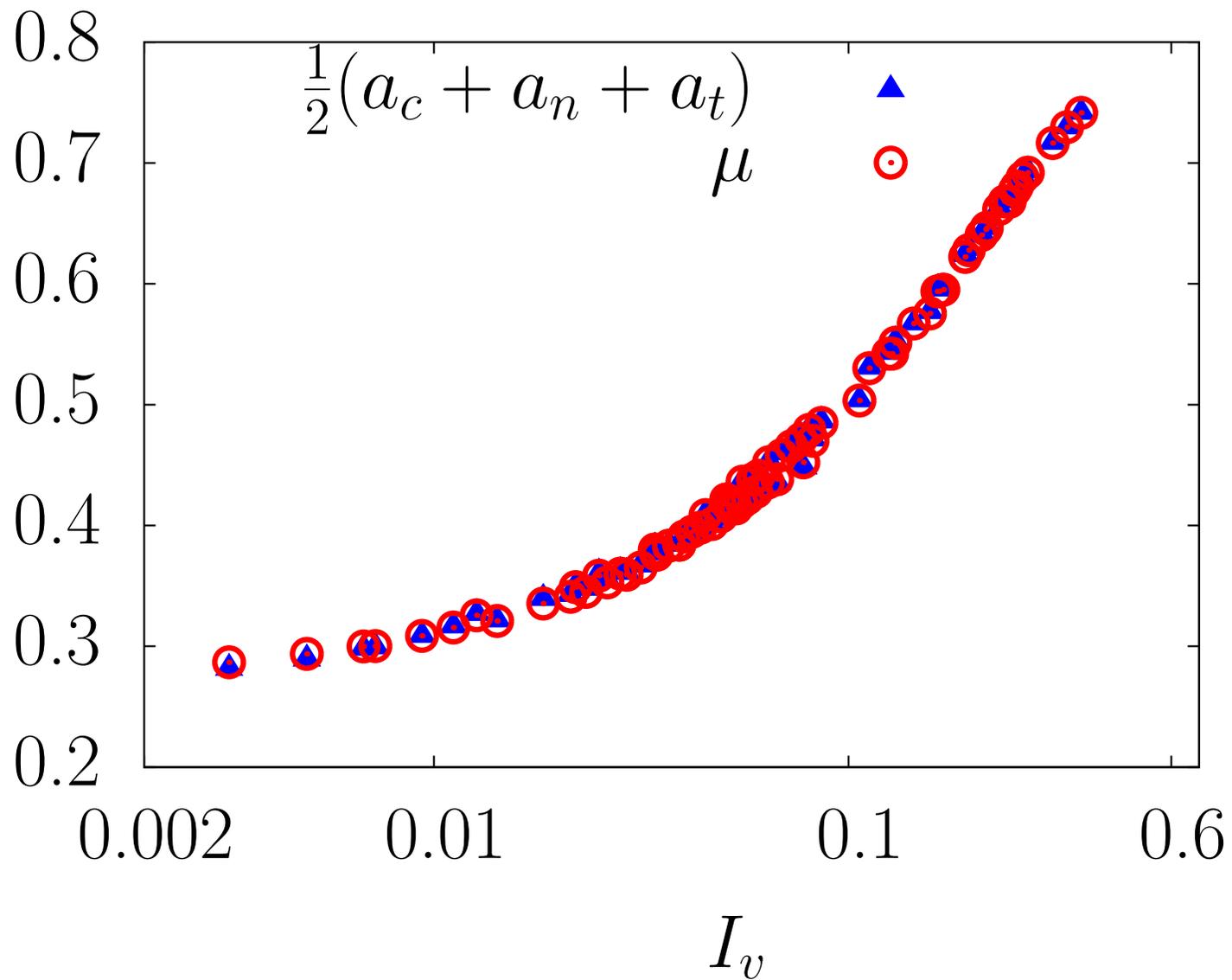
$\sin \varphi$



$$\varepsilon_q \equiv \int (\dot{\varepsilon}_{yy} - \dot{\varepsilon}_{xx}) dt$$

Radjai and Richefeu, Phil. Tran. A (2009)

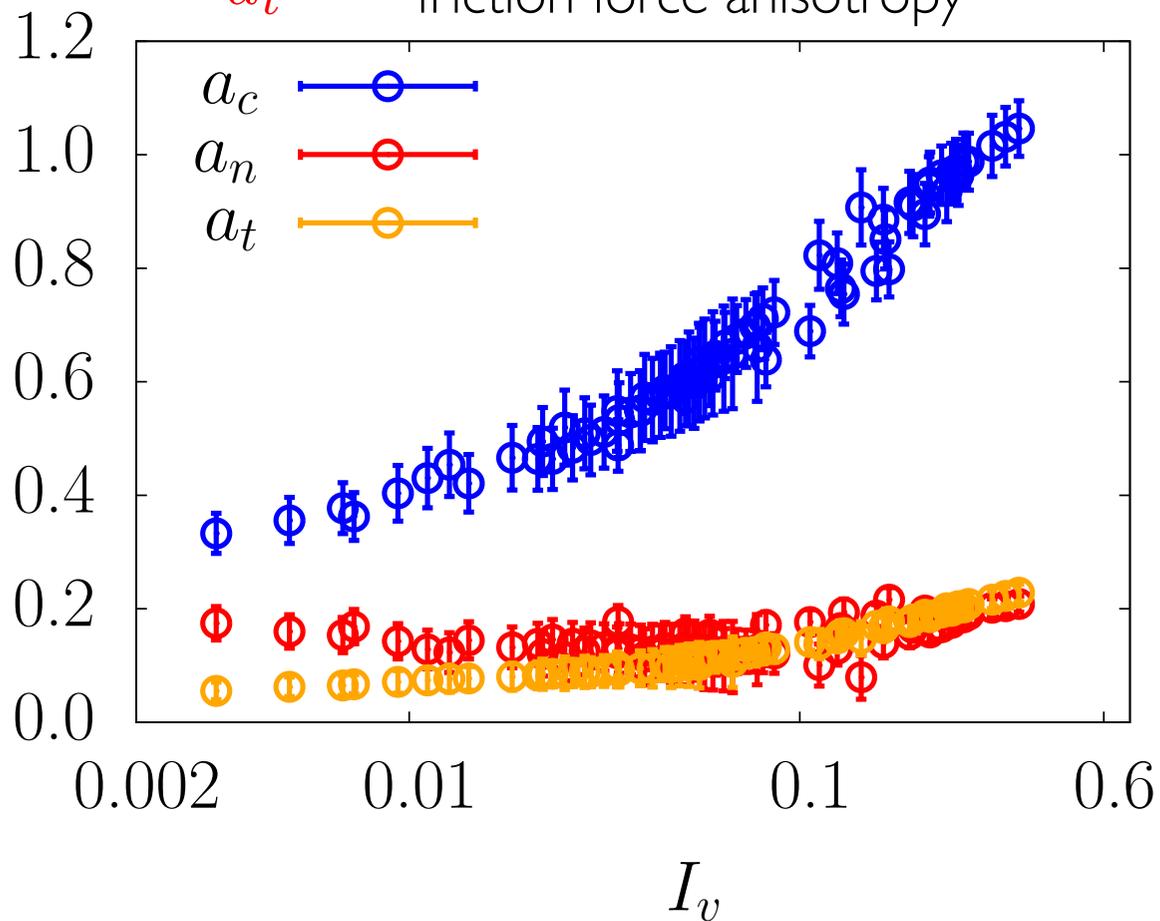




Visco-inertial regime

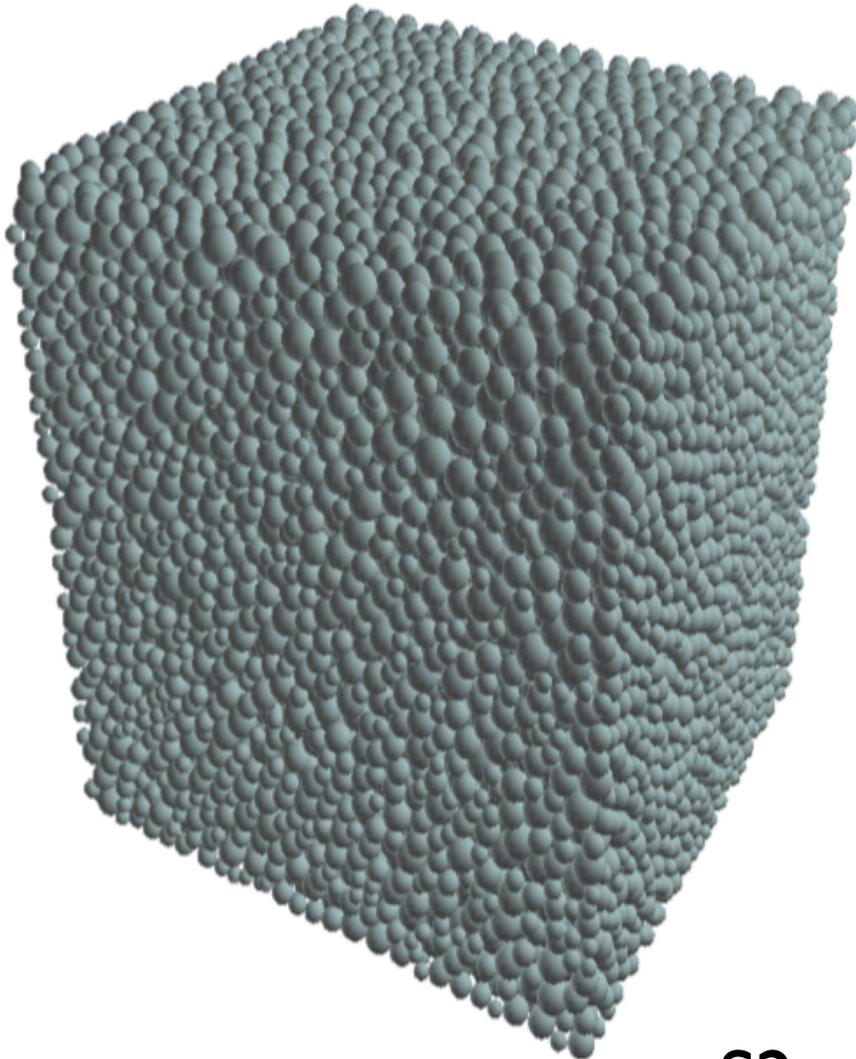
Anisotropies:

- $a_c$  contact network anisotropy
- $a_n$  normal force anisotropy
- $a_t$  friction force anisotropy

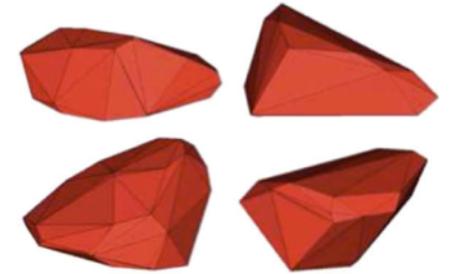


Contact anisotropy is the main origin of shear strength in visco-inertial suspensions. Force chains and friction mobilization play a role at high values of  $I_v$ .

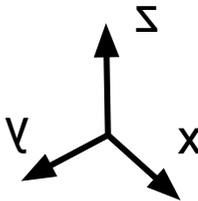
# Application to particle shape effects



S2



S1

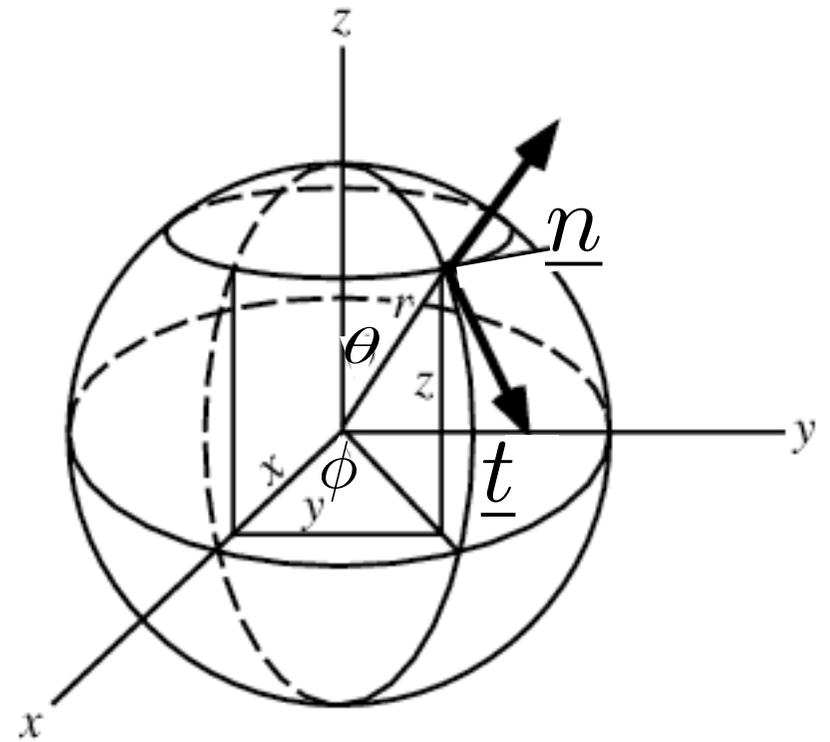


### 3D case

$Y_m^l(\theta, \phi)$  spherical harmonics

Under axisymmetric conditions:

$$Y_0^0 = 1 \quad Y_2^0 = 3 \cos^2 \theta - 1$$



$$P_\Omega(\theta) = \frac{1}{4\pi} \{1 + a (3 \cos^2 \theta - 1)\}$$

$$\Rightarrow \langle \ell \rangle(\theta) = \ell_0 \{1 + a_\ell (3 \cos^2 \theta - 1)\}$$

$$\langle f_n \rangle(\theta) = f_0 \{1 + a_n (3 \cos^2 \theta - 1)\}$$

$$\langle f_t \rangle(\theta) = f_0 a_t \sin 2\theta$$

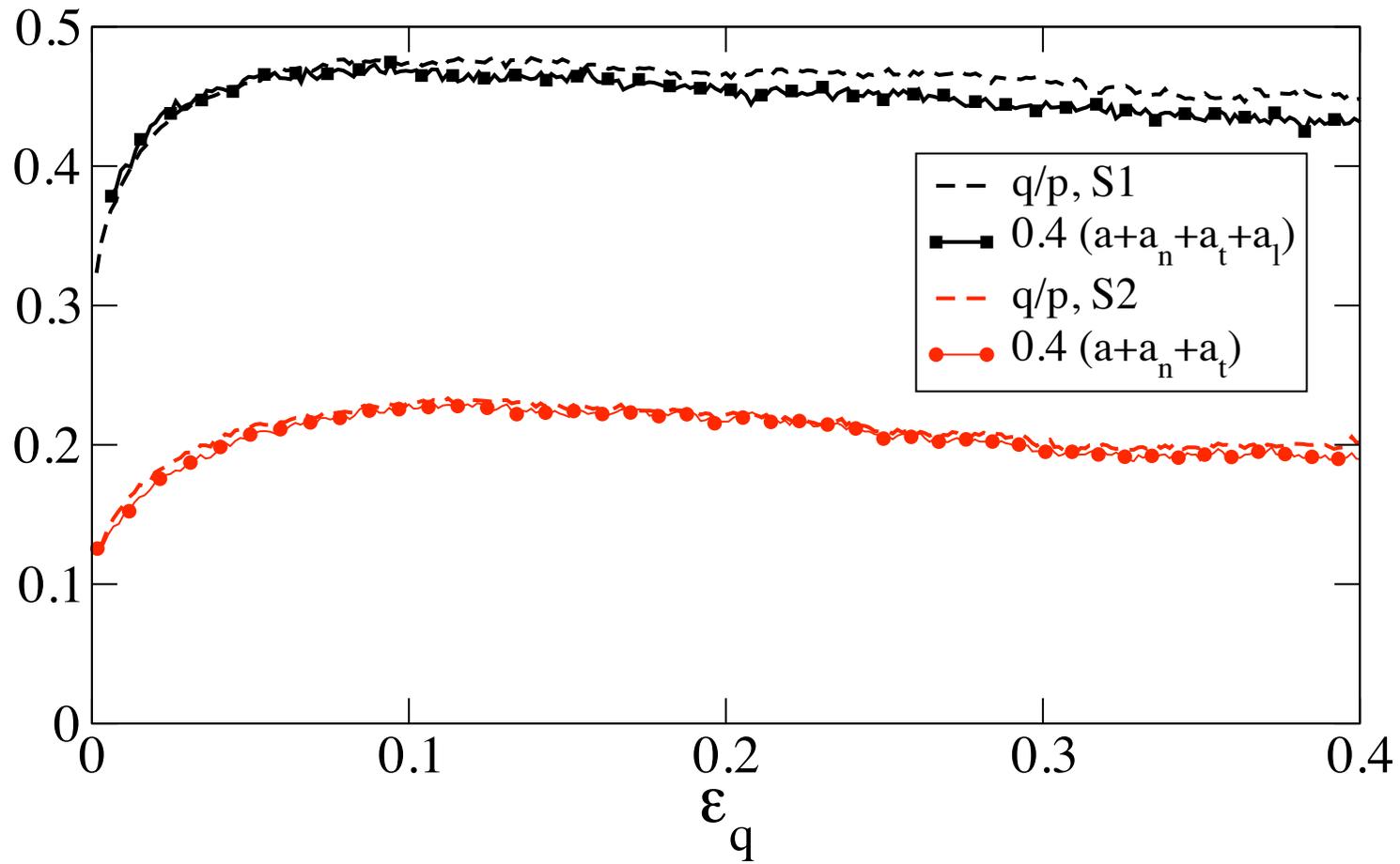
$$\sigma_{\alpha\beta} = n_b \int P_{\Omega f \ell}(\vec{n}, \vec{f}, \ell) \ell(\vec{n}) f_{\beta}(\vec{n}, \ell) n_{\alpha} d\Omega d\vec{f} d\ell$$

with  $d\Omega = \sin \theta d\theta d\phi$

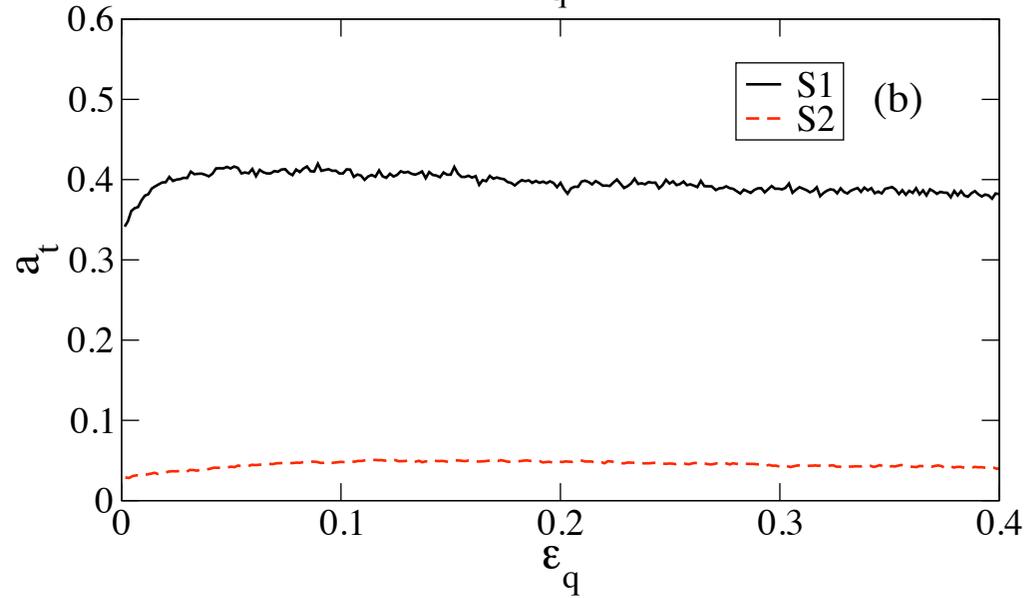
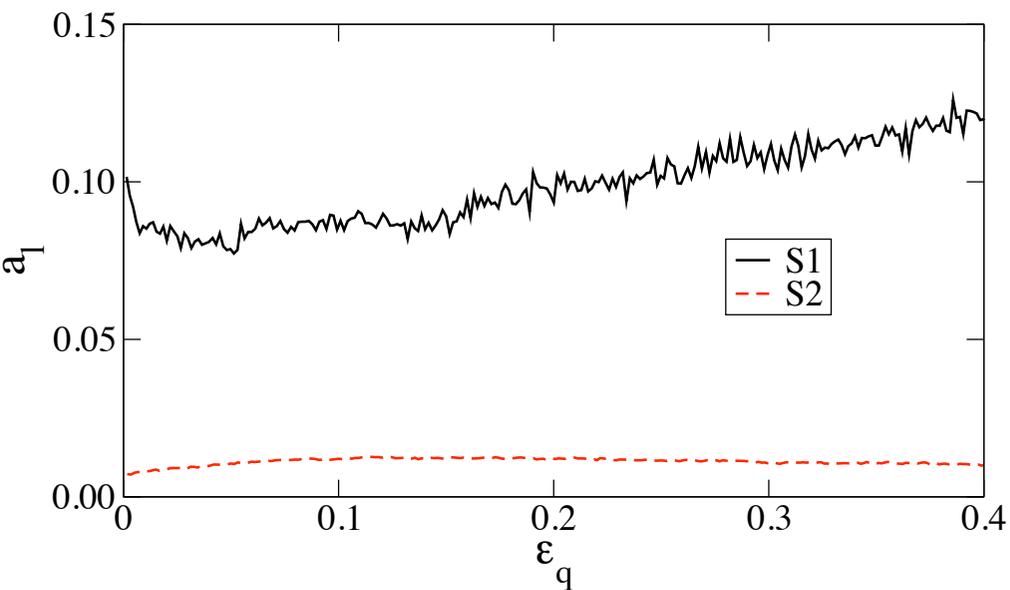
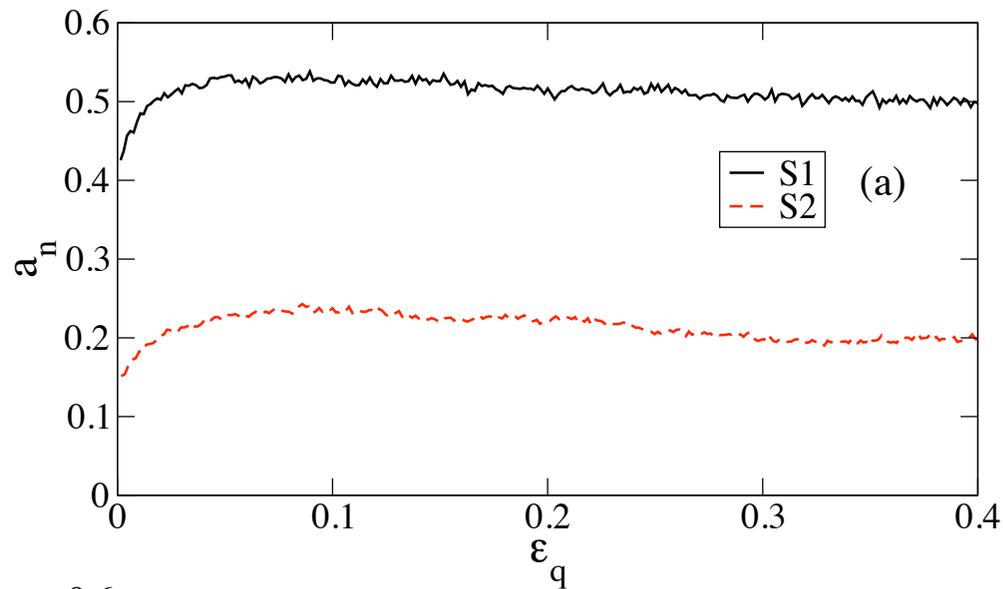
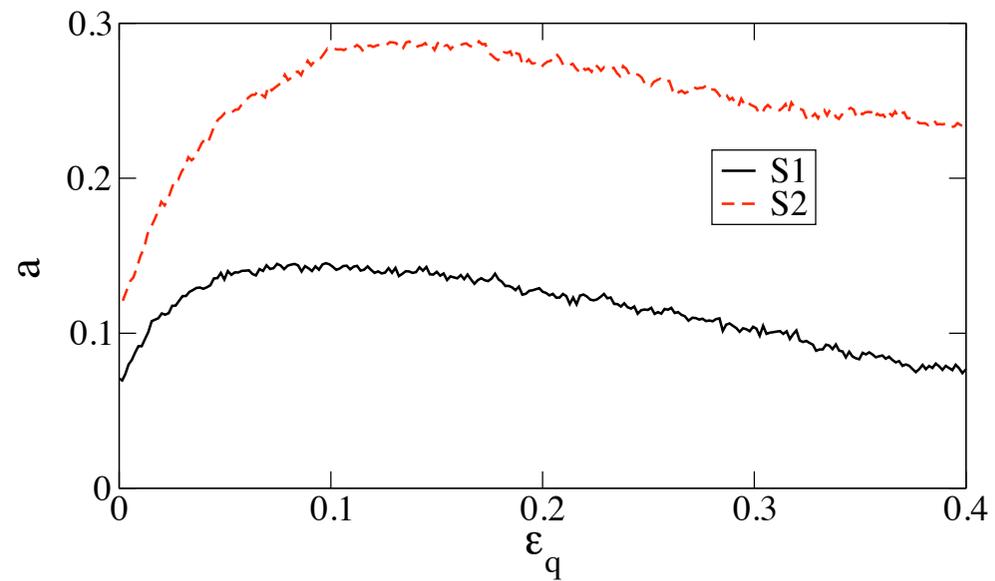
$\Rightarrow$

$$p \simeq n_b \ell_0 f_0$$

$$\frac{q}{p} \simeq \frac{2}{5} (a + a_l + a_n + a_t)$$



E. Azéma, F. Radjai, G. Saussine, Mech. Mat. 41, 2009



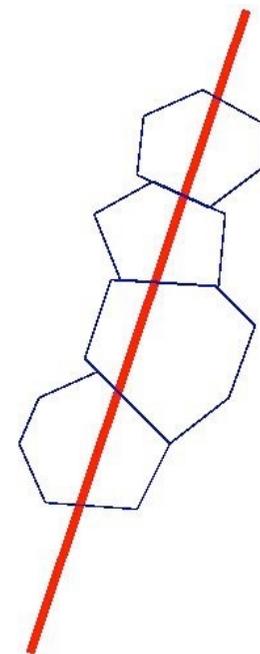
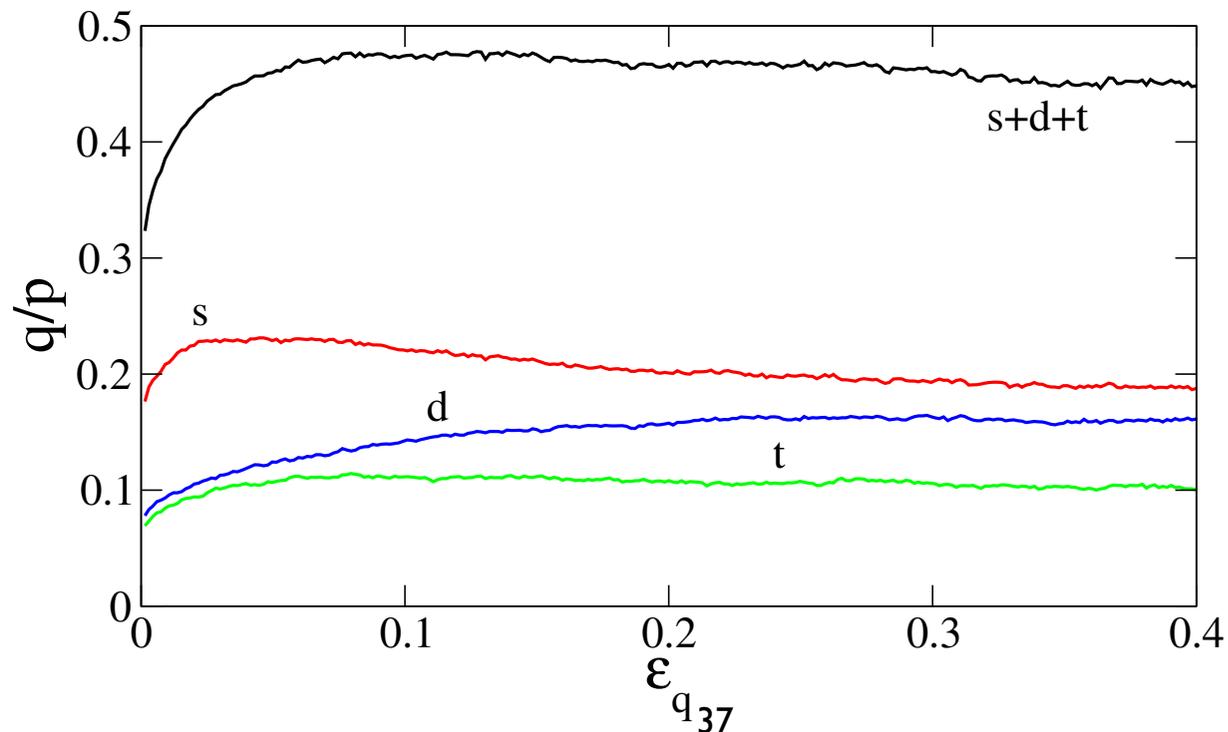
$a_b$  fabric anisotropy

$a_t$  friction mobilization

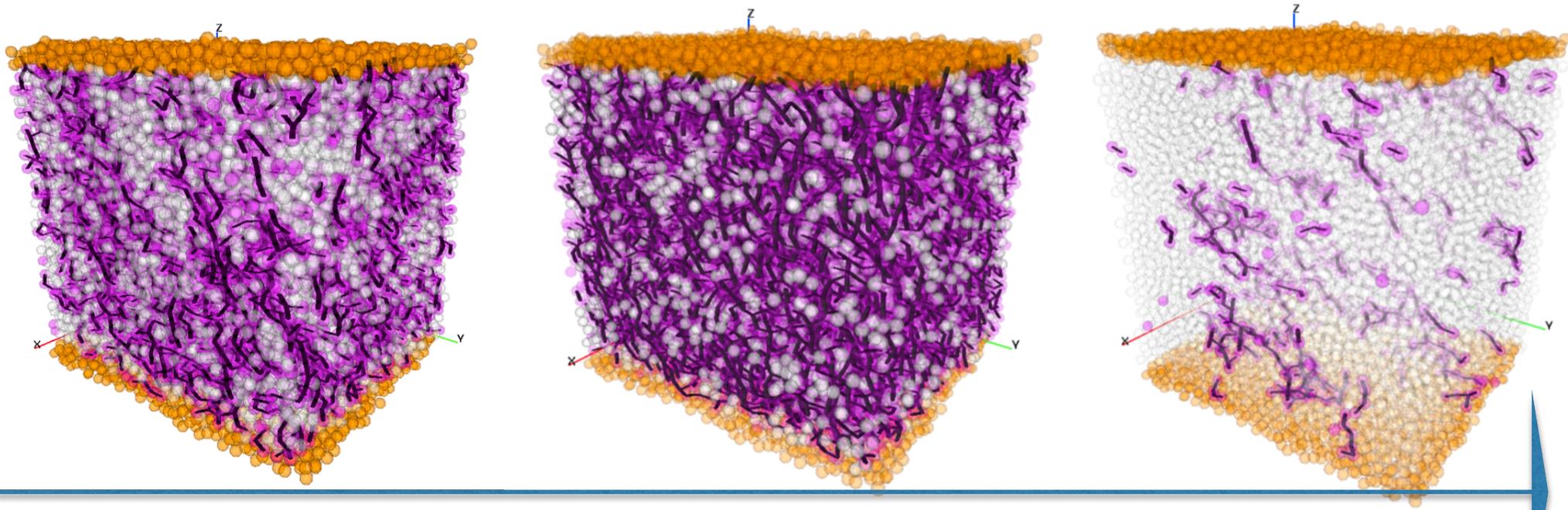
$a_n$  force chains

The effect of aspherical shape is to reinforce force chains (normal force anisotropy) and friction force anisotropy (friction mobilization).

The enhanced force chains and friction mobilization are a consequence of **face-face contacts** (for polyhedra particles).

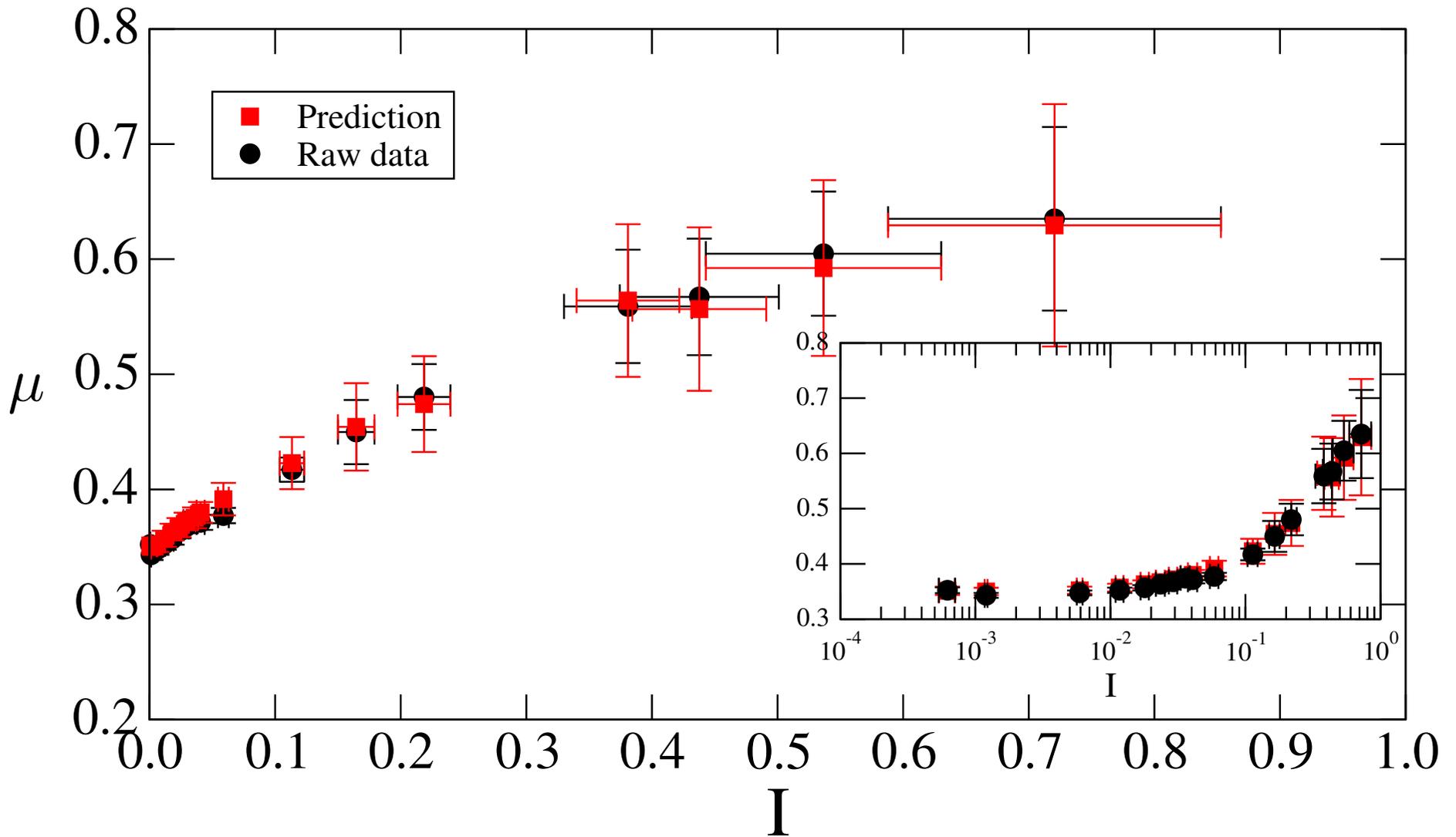


# Application to inertial flows

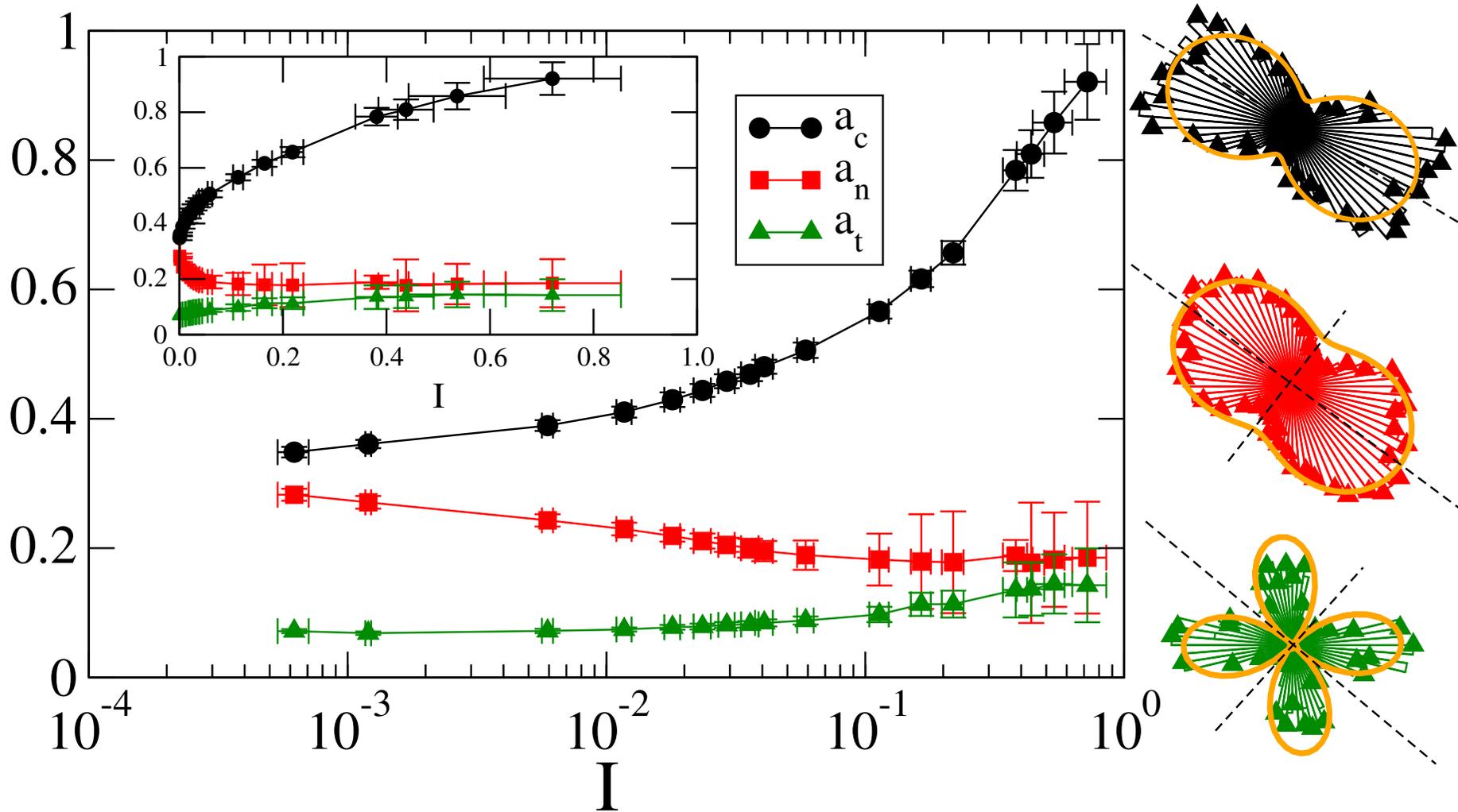


Increasing inertial number

Azéma and Radjai, PRL 112 (2014)



Inertial regime (dry)



Contact anisotropy prevails as inertial forces increase (dry).

## Highlights

The parameter space of granular flows can be reduced.

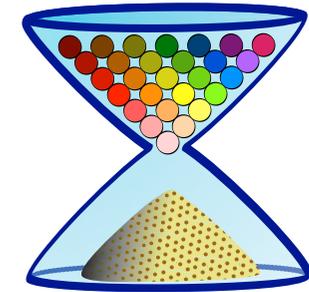
The DEM is a powerful tool when combined with proper analysis.

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