Micromechanics of the elastic behaviour of granular materials

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Overview

- Micromechanics: stress, strain and work
- Discrete Element Simulations
- Variational principles
- Upper and lower bounds; uniform strain and stress
- Statistical theory
- Statistics from DEM simulations
- Conclusions

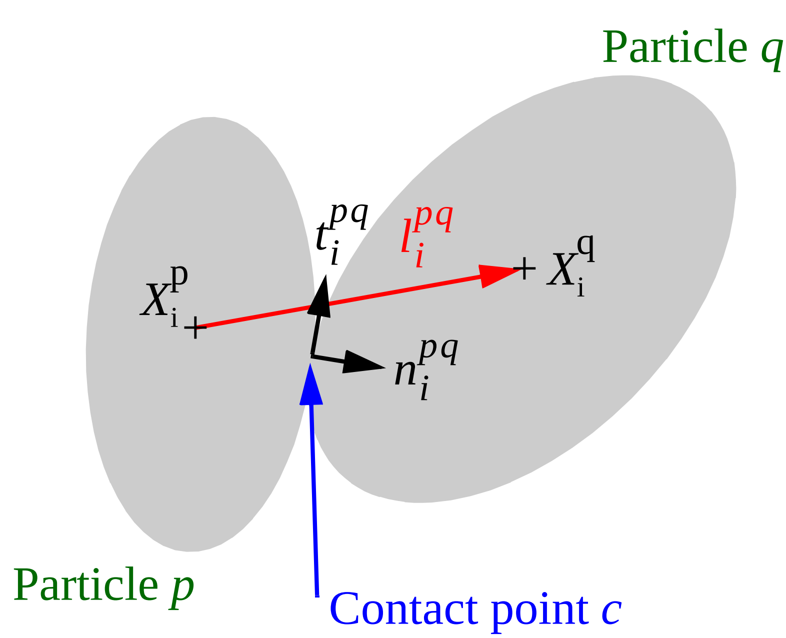
Micromechanics

Objective: relation macroscopic and microscopic characteristics

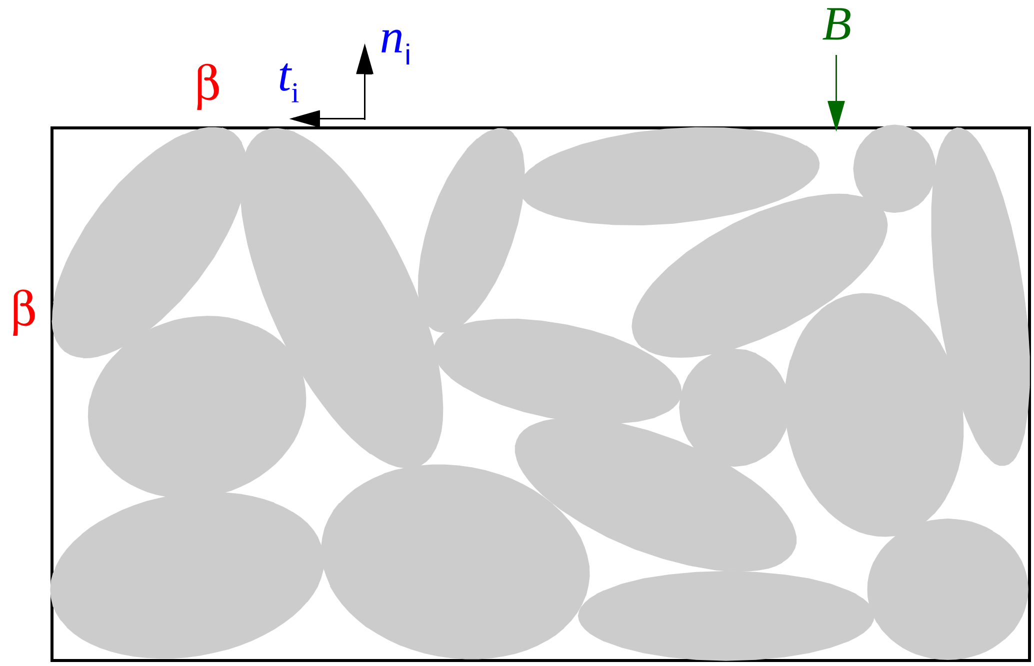
Macroscopic level	Microscopic level
• stress	• contact force
• strain	• contact relative displacement

$$\Delta_i^{pq} = u_i^q - u_i^p$$

Contact geometry



Stress



In boundary terms

$$\bar{\sigma}_{ij} = \frac{1}{S}\int_S \sigma_{ij} dS = \frac{1}{S}\int_S \frac{\partial}{\partial x_k}(x_i \sigma_{kj}) dS$$

$$= \frac{1}{S}\int_B n_k x_i \sigma_{kj} dS = \frac{1}{S}\sum_{\beta \in B} X_i^{\beta} f_j^{\beta}$$

In contact terms

Equilibrium conditions $$\sum_q f_j^{pq} + f_j^{\beta} = 0$$

$$\sum_p \sum_q X_i^p f_j^{pq} + \sum_{\beta \in B} X_i^{\beta} f_j^{\beta} = 0$$

$$\sum_{\beta \in B} f_j^{\beta} x_i^{\beta} = \sum_{c \in S} f_j^c l_i^c$$

Micromechanical stress

$$\bar{\sigma}_{ij} = \frac{1}{S} \sum_{c \in S} f_j^c l_i^c$$

Strain

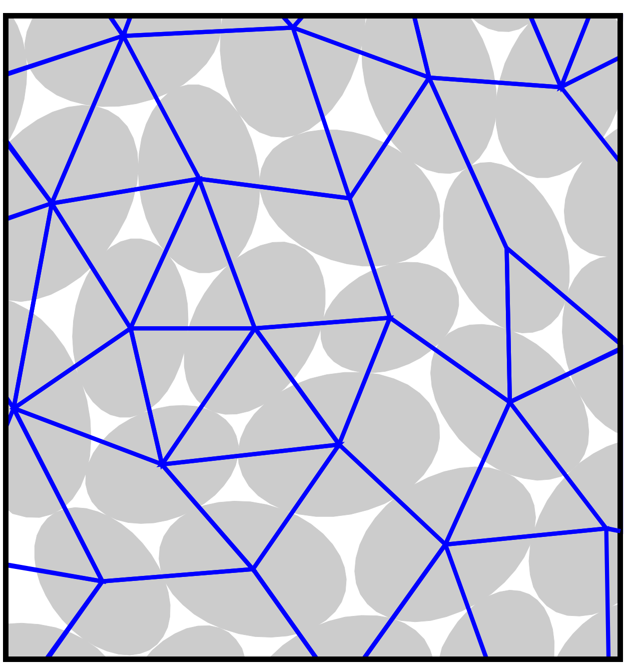
In boundary terms

$$\bar{\alpha}_{ij} = \frac{1}{S}\int_S \frac{\partial u_i}{\partial x_j} dS = \frac{1}{S}\int_B u_i n_j ds = e_{jk}\frac{1}{S}\int_B u_i t_k ds$$

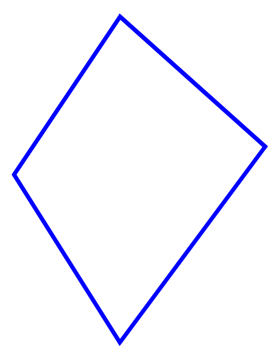
$$= e_{jk}\frac{1}{S}\int_B u_i \frac{dx_k}{ds} ds = -e_{jk}\frac{1}{S}\int_B \frac{du_i}{ds} x_k ds = -e_{jk}\frac{1}{S}\sum_{\alpha \in B} \Delta_i^{\alpha} X_k^{\alpha}$$

In contact terms

Compatibility conditions $\sum_s \Delta_i^{rs} + \Delta_i^{r\alpha} = 0$



Network connecting particle centres

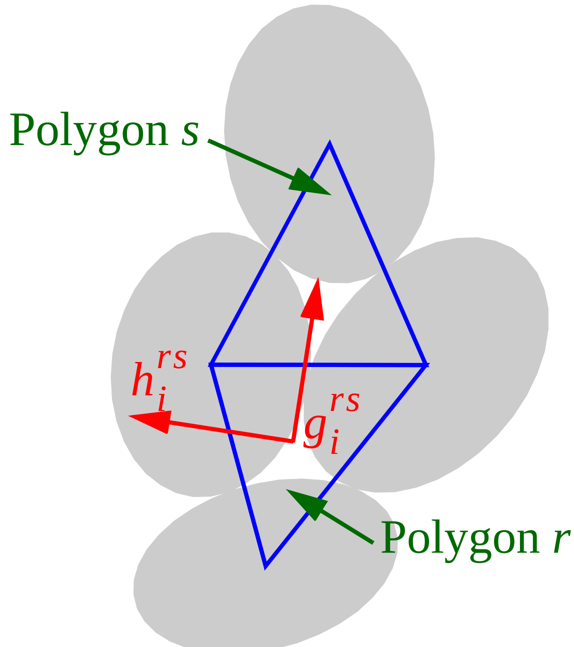


$$\sum_r \sum_s \Delta_i^{rs} X_j^r + \sum_r \Delta_i^{r\alpha} X_j^r = 0$$

$$\sum_{\alpha \in B} \Delta_i^{\alpha} X_j^{\alpha} = \sum_{c \in S} \Delta_i^c g_j^c$$

$$\bar{\alpha}_{ij} = \frac{1}{S} \sum_{c \in S} \Delta_i^c h_j^c$$

$$h_j^c = -e_{jk} g_k^c$$



Work

$$\frac{1}{S} \sum_{c \in S} f_i^c \Delta_i^c = \sigma_{ij} \varepsilon_{ij}$$

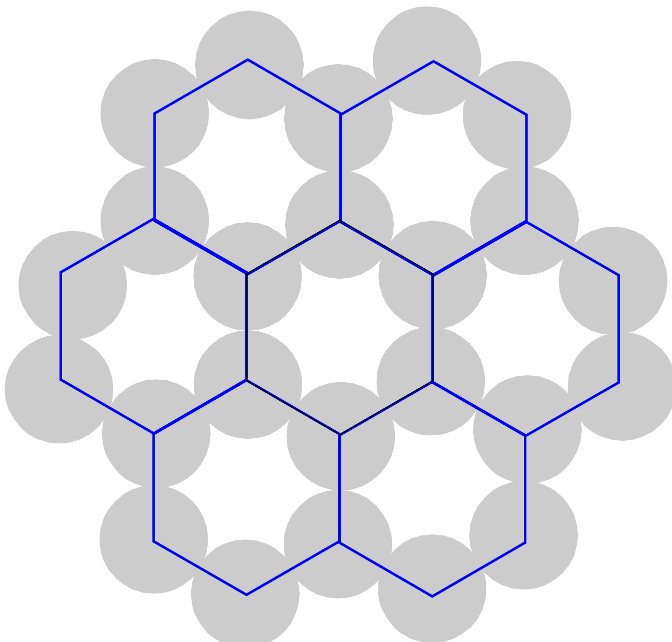
Geometry

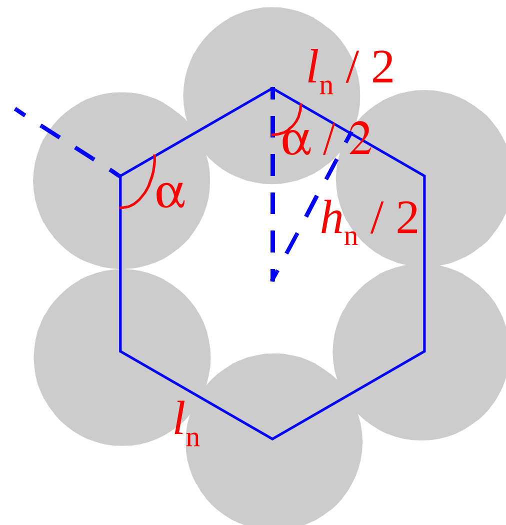
$$\delta_{ij} = \frac{1}{S} \sum_{c \in S} l_i^c h_j^c$$

Uniform strain and stress

$$\Delta_i^c = \varepsilon_{ij} l_j^c \qquad f_i^c = \sigma_{ij} h_j^c$$

Geometrical considerations

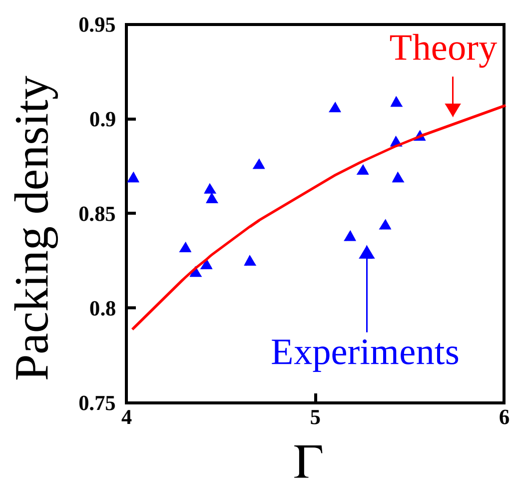




Coordination number $\Gamma = 3$

$$\alpha = \frac{2\pi}{\Gamma} \qquad \tan\frac{\alpha}{2} = \frac{h_n}{l_n}$$

$$\text{Packing density} \cong \frac{\pi}{\Gamma \tan\frac{\pi}{\Gamma}}$$



Summary of micromechanics

Particle	Connecting relation	Polygon
$\sum_q h_i^{pq} = 0$	$\delta_{ij} = \frac{1}{S} \sum_{c \in S} h_i^c l_j^c$	$\sum_s l_i^{rs} = 0$
$\sum_q f_i^{pq} = 0$	$f_i^c = S_{ij}^c \Delta_j^c$	$\sum_s \Delta_i^{rs} = 0$
$\sigma_{ij} = \frac{1}{S} \sum_{c \in S} f_i^c l_j^c$	$\sigma_{ij}\varepsilon_{ij} = \frac{1}{S} \sum_{c \in S} f_i^c \Delta_i^c$	$\varepsilon_{ij} = \frac{1}{S} \sum_{c \in S} \Delta_i^c h_j^c$

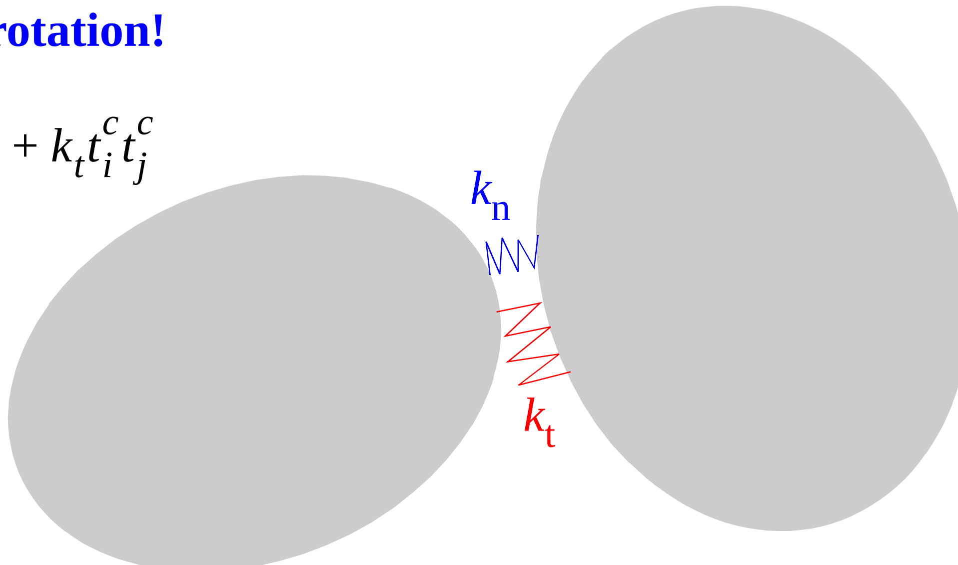
Elastic contact constitutive relation

No particle rotation!

$$S_{ij}^c = k_n n_i^c n_j^c + k_t t_i^c t_j^c$$

$$f_n^c = k_n \Delta_n^c$$

$$f_t^c = k_t \Delta_t^c$$



Discrete Element Method simulations

- isotropic assemblies with 50,000 disks
- wide lognormal PSD
- coordination numbers $4 \le \Gamma \le 6$
- stiffness ratios $0 \le k_t / k_n \le 1$
- periodic boundaries
- compressive and shearing loading

Extremum principles

Minimum potential energy principle

$f^*{}_i^c$, $\Delta^*{}_i^c$ compatible, no equilibrium

f_i^c, Δ_i^c compatible, equilibrium

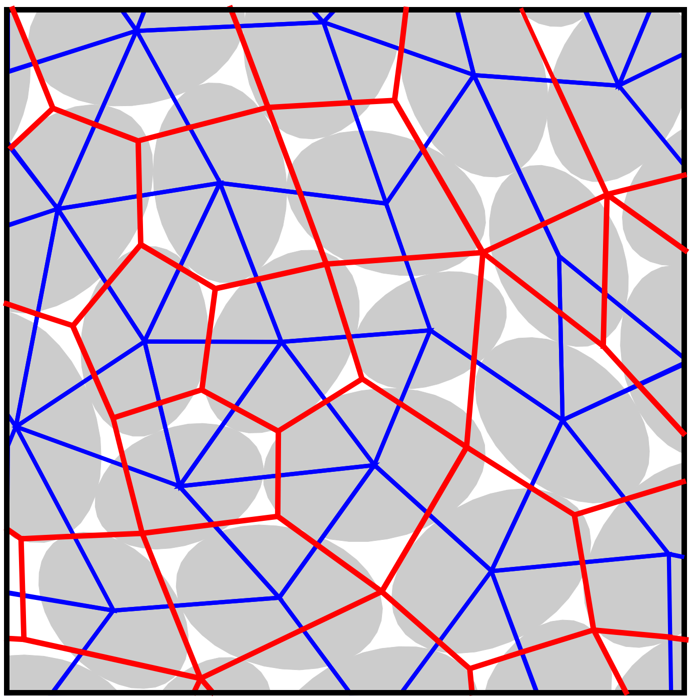
$$\frac{1}{2}\sum_{c \in S} f_i^c \Delta_i^c \le \frac{1}{2}\sum_{c \in S} f^*{}_i^c \Delta^*{}_i^c$$

Minimum complementary energy principle

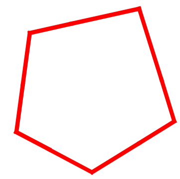
$f^*{}_i^c$, $\Delta^*{}_i^c$ equilibrium, not compatible

f_i^c, Δ_i^c equilibrium, compatible

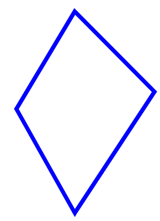
Then $\frac{1}{2}\sum_{c \in S} f^*{}_i^c \Delta^*{}_i^c \le \frac{1}{2}\sum_{c \in S} f_i^c \Delta_i^c$



Network connecting polygon centres



Network connecting particle centres



Take $\Delta^{*c}_i = \varepsilon_{ij} l^c_j$: uniform strain

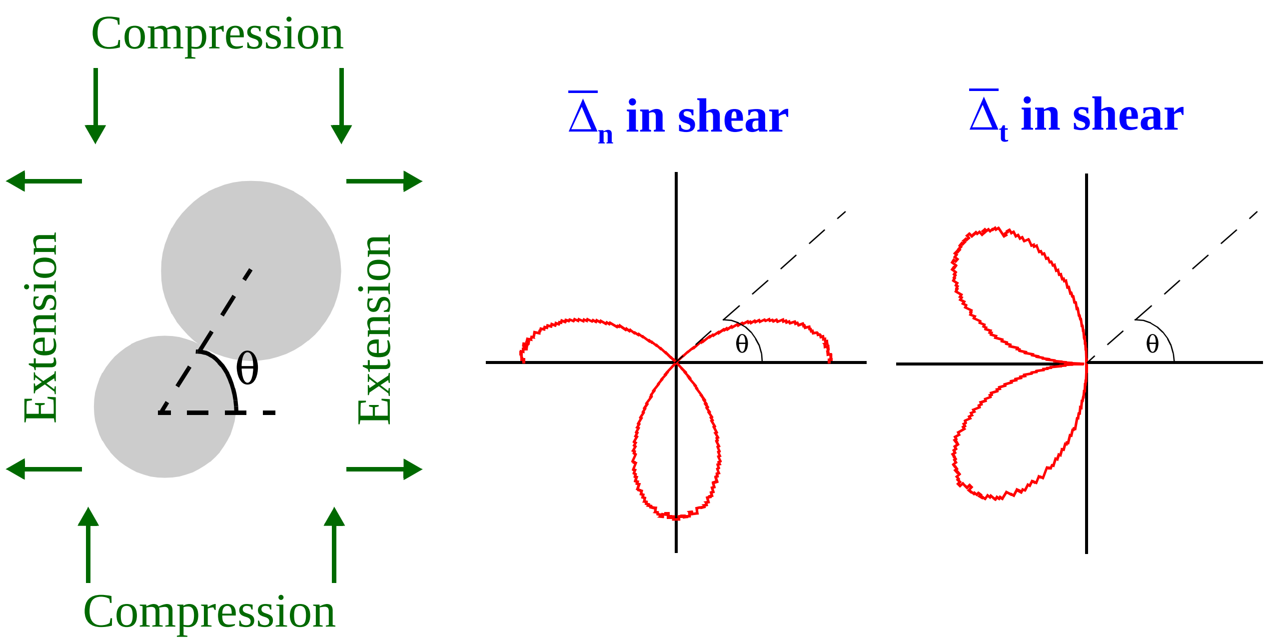
Upper bound $\varepsilon_{ij} L_{ijkl} \varepsilon_{kl} \leq \varepsilon_{ij} L^{\varepsilon}_{ijkl} \varepsilon_{kl} \equiv \varepsilon_{ij} \left(\frac{1}{S} \sum_{c \in S} S^c_{ik} l^c_j l^c_l \right) \varepsilon_{kl}$

Take $f^{*c}_i = \sigma_{ij} h^c_j$: uniform stress

Lower bound $\sigma_{ij} M_{ijkl} \sigma_{kl} \leq \sigma_{ij} M^{\sigma}_{ijkl} \sigma_{kl} \equiv \sigma_{ij} \left(\frac{1}{S} \sum_{c \in S} S^{-1c}_{ik} h^c_j h^c_l \right) \sigma_{kl}$

Orientational averaging

Uniform strain $\Delta_i = \varepsilon_{ij} l_j$



Contact distribution

$$\sigma_{ij} = \frac{1}{S}\sum_{c \in S} f_j^c l_i^c = \frac{M}{S}\sum_{\theta_g} E(\theta_g)\Delta\theta \overline{f_j l_i}(\theta_g) = m_S \int_0^{2\pi} E(\theta)\overline{f_j l_i}(\theta) d\theta$$

Contact density

Overall average $\langle w(\theta) \rangle = m_S \int_0^{2\pi} E(\theta)\overline{w(\theta)} d\theta$

Statistical potential energy principle

Minimize potential energy $\langle \frac{1}{2}\Delta_i S_{ij}\Delta_j \rangle$

Subject to constraints $\varepsilon_{ij} = \langle \Delta_i h_j \rangle \qquad \langle f_i \Delta_i \rangle = \sigma_{ij}\varepsilon_{ij}$

Gaussian distributions
$$\overline{\Delta_n^2(\theta)} = \overline{\Delta_n(\theta)}^2 + \sigma_n^2(\theta)$$
$$\overline{\Delta_t^2(\theta)} = \overline{\Delta_t(\theta)}^2 + \sigma_t^2(\theta)$$

Disorder $\chi \equiv \langle k_n \sigma_n^2 + k_t \sigma_t^2 \rangle = \alpha(1-\alpha)\varepsilon_{ij}(L_{ijkl}^{\varepsilon} - L_{ijkl}^{\sigma})\varepsilon_{kl}$

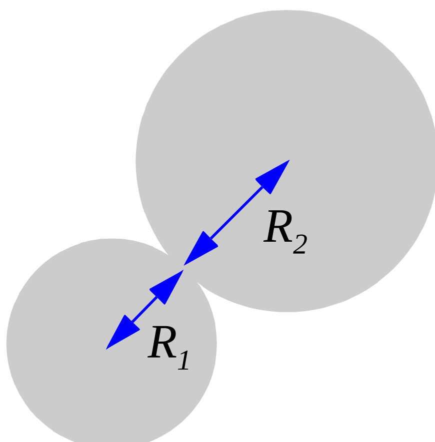
Choose α for *maximum* disorder, then

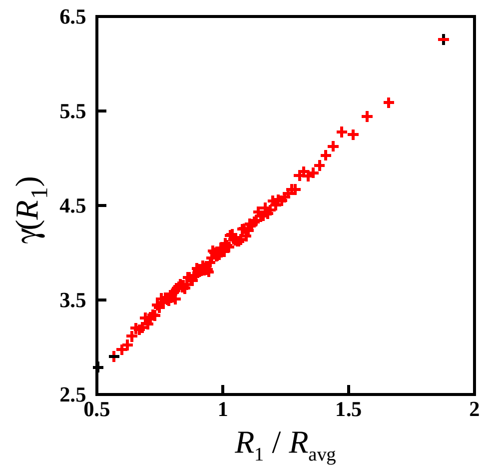
$$L_{ijkl} = \frac{L_{ijkl}^{\varepsilon} + L_{ijkl}^{\sigma}}{2}$$

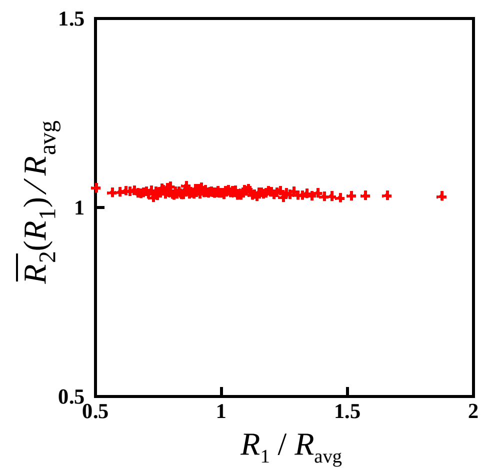
Observations from DEM simulations

Geometry

Loose system $\overline{l}_n > 2R_{\mathrm{avg}}$





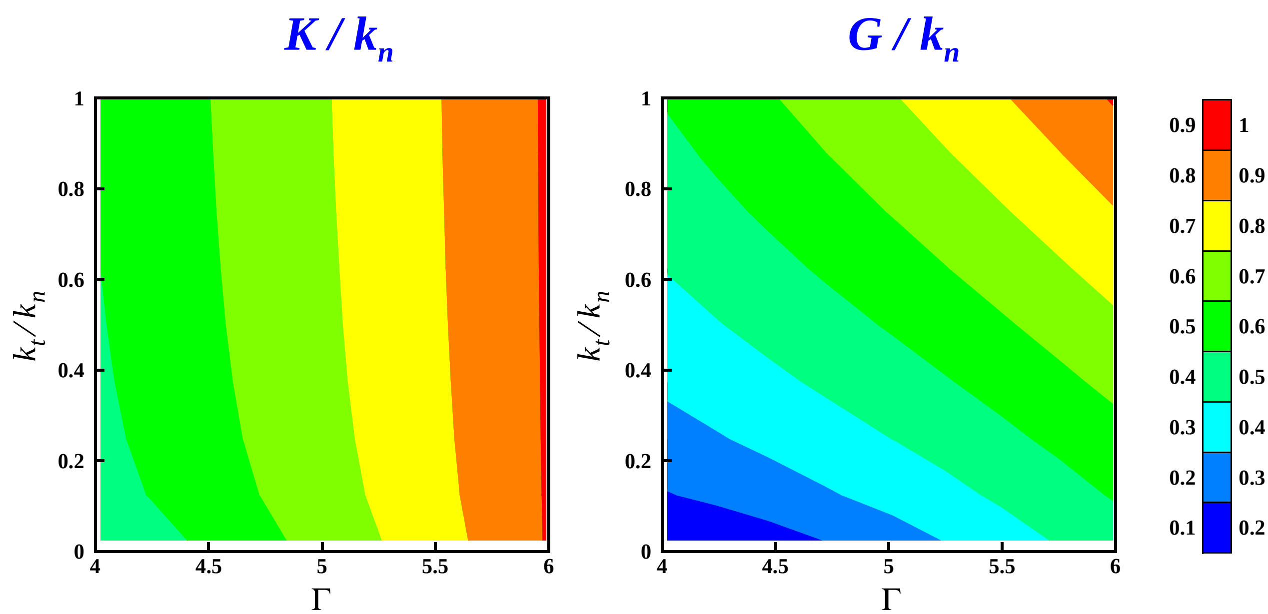


Large particles have more contacts

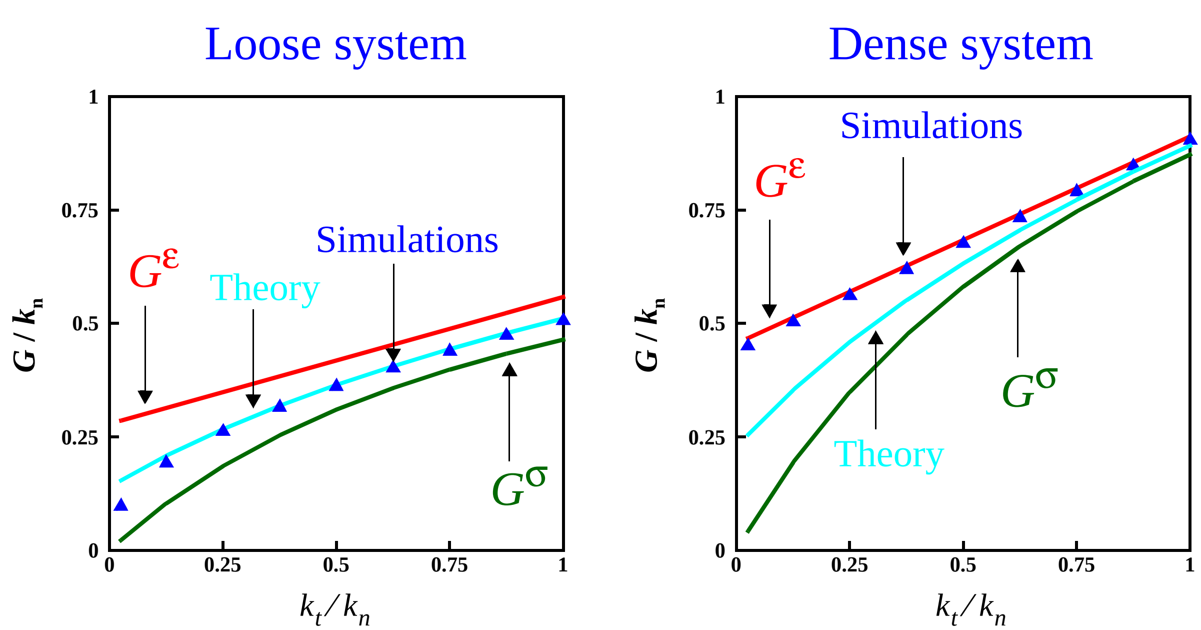
No size preference

Moduli

Simulations

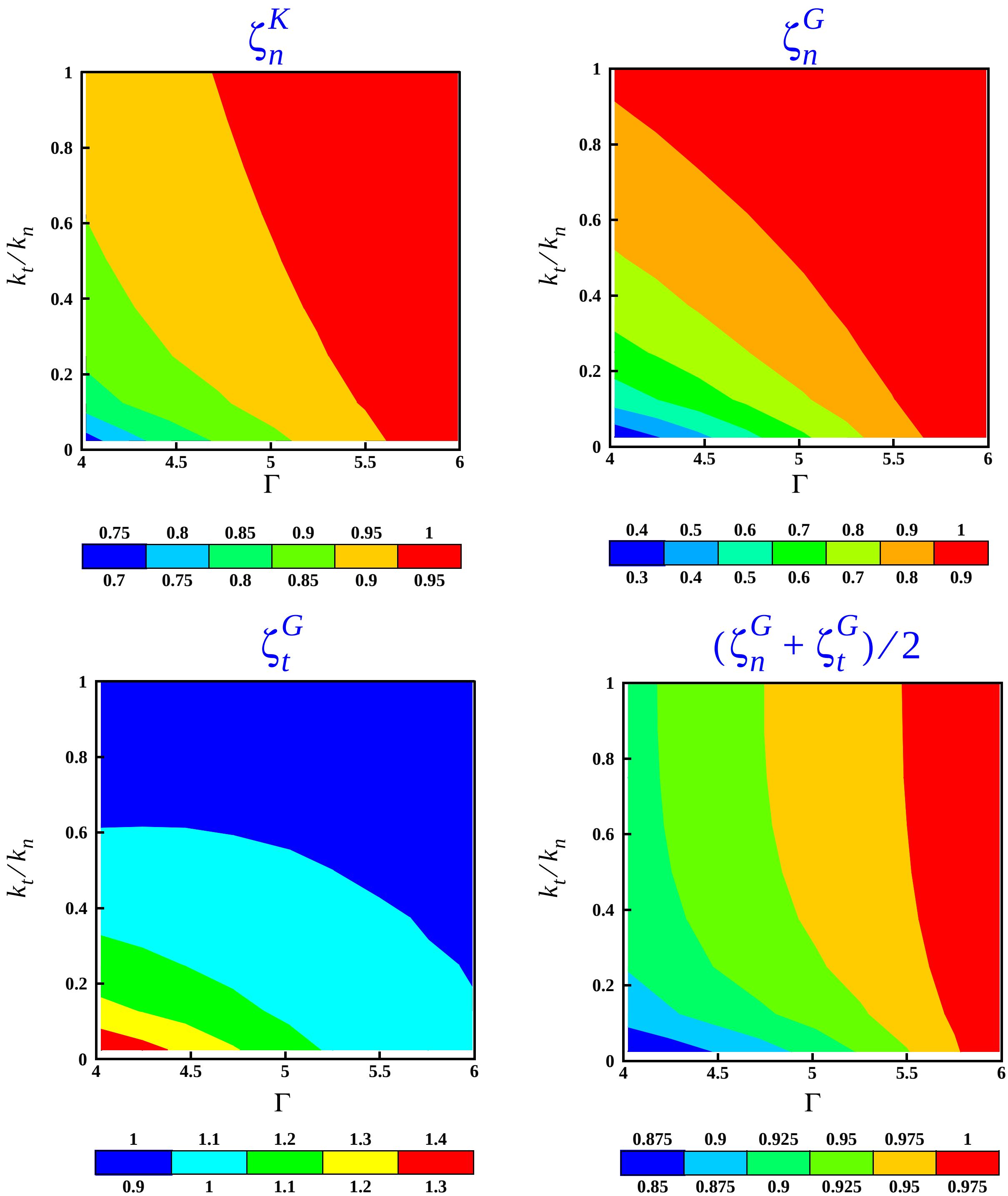


Comparison of theory and simulations



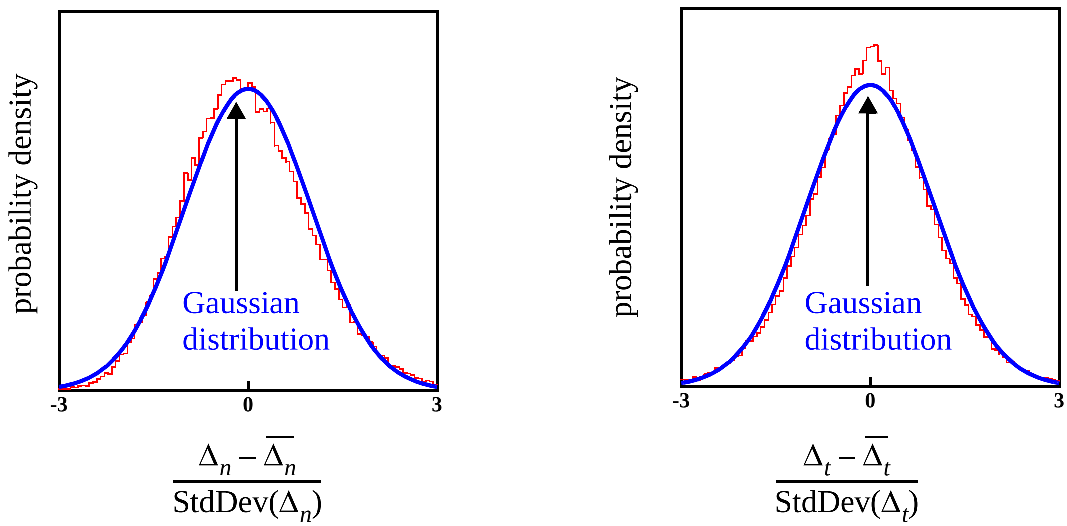
Displacements

$$\overline{\Delta}_i = \zeta \varepsilon_{ij} \bar{l}_j$$

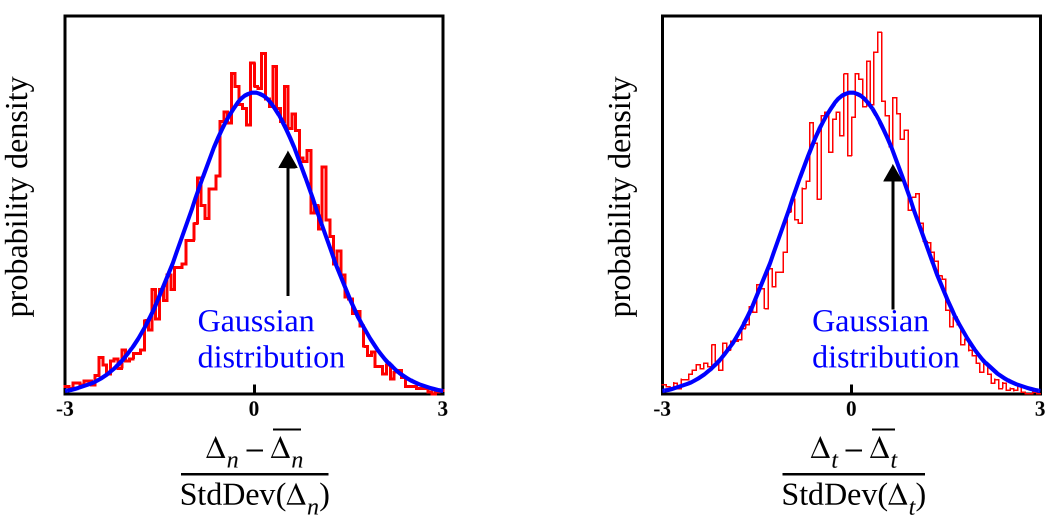


Probability density functions

Compression



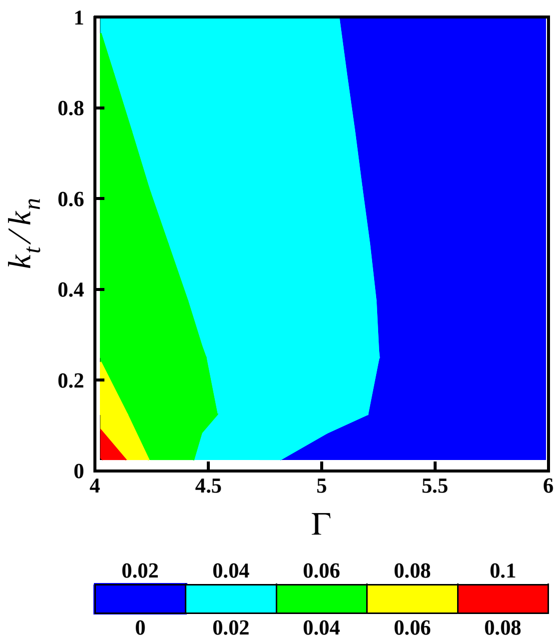
Shear



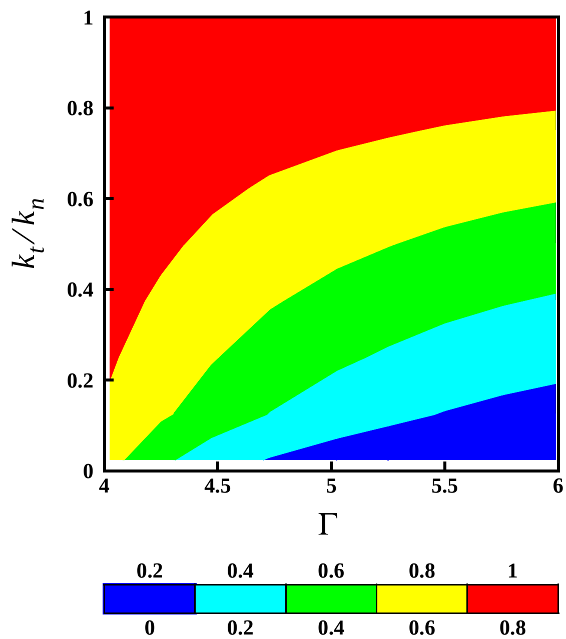
Energy ratios

$$E_n = \frac{1}{2}\langle k_n \overline{\Delta_n^2} \rangle \qquad E_n = \frac{1}{2}\langle k_t \overline{\Delta_t^2} \rangle$$

E_t / E_n in compression



E_t / E_n in shear



Conclusions

- two regimes: uniform strain and uniform stress
- upper and lower bound for moduli
- uniform strain assumption is only correct for dense systems
- statistical theory gives average of uniform strain and stress; appropriate for loose systems
- Gaussian probability functions for normal and tangential components of relative displacements
- no equipartition of energy

Uniform field moduli

$$\frac{K^{\varepsilon}}{k_n} = \frac{m_S}{4}\overline{l_n^2} \qquad \frac{G^{\varepsilon}}{k_n} = \frac{m_S}{8}\left(1 + \frac{k_t}{k_n}\right)\overline{l_n^2}$$

$$\frac{K^{\sigma}}{k_n} = \frac{k_t/k_n}{m_S(\lambda\overline{h_n^2} + \overline{h_t^2})} \qquad \frac{G^{\sigma}}{k_n} = \frac{2k_t/k_n}{m_S(1 + k_t/k_n)(\overline{h_n^2} + \overline{h_t^2})}$$

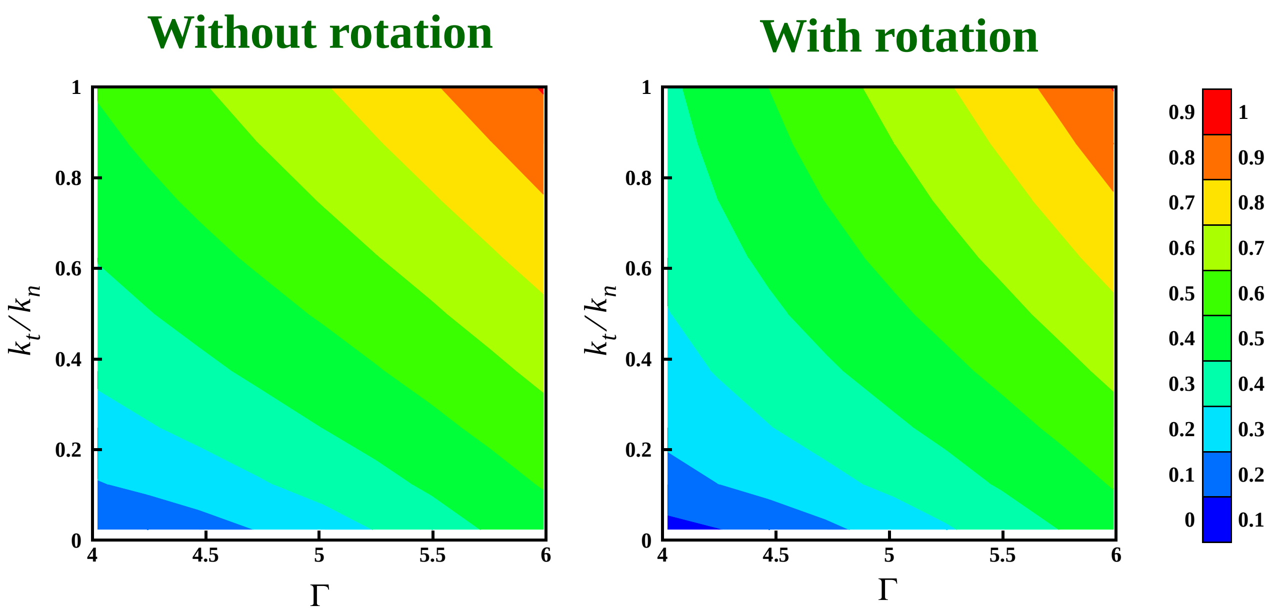
Theoretical generalised strain

$$\zeta_n^K = \frac{1}{2} + \frac{K^{\sigma}}{k_n}\frac{\overline{h_n}}{\overline{l_n}}$$ Compression

$$\zeta_n^G = \frac{1}{2} + \frac{G^{\sigma}}{k_n}\frac{\overline{h_n}}{\overline{l_n}}$$ Shear

$$\zeta_t^G = \frac{1}{2} + \frac{G^{\sigma}}{k_t}\frac{\overline{h_n}}{\overline{l_n}}$$ Shear

Influence of rotation; shear modulus



Particle size distribution