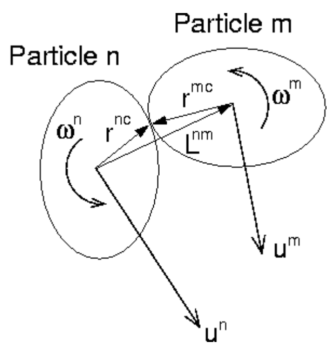
Enhanced continuum models derived from random discrete particle structures



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Introduction

- Research done in collaboration with:
  - Ching Chang (University of Massachusetts)
  - René de Borst (TU Delft)

- Derivation of enhanced continuum models from random, discrete granular structure (homogenisation)

- Enhanced continua better describe *heterogeneous* responses of particle assemblies, as occurring for
  - narrow failure zones (shear bands)
  - high-frequency wave propagation

- Research is focused towards *elastic behaviour* of granular materials

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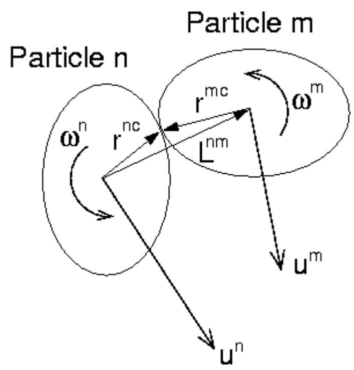
Kinematics of two particles in contact



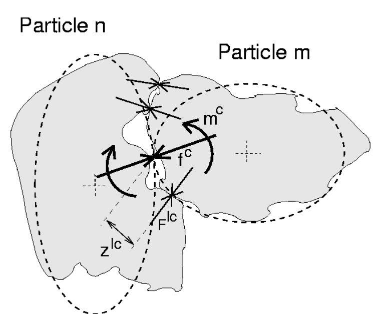
$$\Delta u_i^c = \Delta u_i^{nm} = u_i^m - u_i^n + e_{ijk}\left(\omega_j^m r_k^{mc} - \omega_j^n r_k^{nc}\right)$$

$$\Delta \omega_i^c = \Delta \omega_i^{nm} = \omega_i^m - \omega_i^n$$

Kinematics of two convex-shaped particles

Constitutive laws at particle contact

- Force-displacement contact relation: $f_i^c = K_{ij}^c \Delta u_j^c$
- Moment-rotation contact relation: $m_i^c = G_{ij}^c \Delta \omega_j^c$

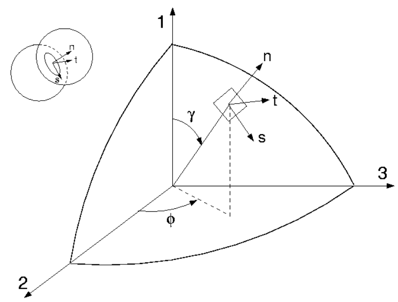


Representation arbitrarily-shaped particles by convex-shaped particles

- Stiffness tensors:

$$K_{ij}^{c} = K_{ij}^{nm} = Kn\ n_i^c n_j^c + Ks\ s_i^c s_j^c + Kt\ t_i^c t_j^c$$

$$G_{ij}^{c} = G_{ij}^{nm} = Gn\ n_i^c n_j^c + Gs\ s_i^c s_j^c + Gt\ t_i^c t_j^c$$



$$\mathbf{n}^c = \cos\gamma\ \mathbf{e}_1 + \sin\gamma\cos\phi\ \mathbf{e}_2 + \sin\gamma\sin\phi\ \mathbf{e}_3$$

$$\mathbf{s}^c = -\sin\gamma\ \mathbf{e}_1 + \cos\gamma\cos\phi\ \mathbf{e}_2 + \cos\gamma\sin\phi\ \mathbf{e}_3$$

$$\mathbf{t}^c = \mathbf{n}^c \times \mathbf{s}^c = -\sin\varphi\ \mathbf{e}_2 + \cos\phi\ \mathbf{e}_3$$

Local coordinate system at the contact between two particles

From discrete kinematics to continuum kinematics

(Enhanced continuum models: Chang & Liao, 1990; Chang & Ma, 1992; Chang & Gao, 1995; Mühlhaus & Oka, 1996)

- Displacement of particle *n* : $u_i^n \rightarrow \hat{u}_i^n = \hat{u}_i\,(x_p)\big|_{x_p = x_p^n}$
- Rotation of particle *n* : $\omega_i^n \rightarrow \hat{\omega}_i^n = \hat{\omega}_i\,(x_p)\big|_{x_p = x_p^n}$

- Kinematics of neighbouring particle *m* estimated through Taylor approximations:

$$u_i^m \rightarrow \hat{u}_i^m = \hat{u}_i^n + \hat{u}_{i,j}^n L_j^{nm} + \frac{1}{2!}\hat{u}_{i,jk}^n L_j^{nm} L_k^{nm} + \frac{1}{3!}\hat{u}_{i,jkl}^n L_j^{nm} L_k^{nm} L_l^{nm} + \ldots$$

$$\omega_i^m \rightarrow \hat{\omega}_i^m = \hat{\omega}_i^n + \hat{\omega}_{i,j}^n L_j^{nm} + \frac{1}{2!}\hat{\omega}_{i,jk}^n L_j^{nm} L_k^{nm} + \frac{1}{3!}\hat{\omega}_{i,jkl}^n L_j^{nm} L_k^{nm} L_l^{nm} + \ldots$$

with the branch vector:

$$L_i^c = L_i^{nm} = r_i^{nc} - r_i^{mc}$$

Various continua

- Standard Boltzmann continuum :

$$\Delta u_i^c = F_1\left(\hat{u}_{i,j}^n\right) = \hat{u}_{i,j}^n L_j^c$$

- Second-gradient continuum :

$$\Delta u_i^c = F_2\left(\hat{u}_{i,j}^n, \hat{u}_{i,jk}^n, \hat{u}_{i,jkl}^n\right) = \hat{u}_{i,j}^n L_j^c + \frac{1}{2}\hat{u}_{i,jk}^n L_j^c L_k^c + \frac{1}{6}\hat{u}_{i,jkl}^n L_j^c L_k^c L_l^c$$

- Fourth-gradient continuum :

$$\Delta u_i^c = F_3\left(\hat{u}_{i,j}^n, \hat{u}_{i,jk}^n, \hat{u}_{i,jkl}^n, \hat{u}_{i,jklm}^n, \hat{u}_{i,jklmn}^n\right) = \ldots$$

- Cosserat continuum :

$$\Delta u_i^c = F_4\left(\hat{u}_{i,j}^n, \hat{\omega}_k^n\right) = \left(\hat{u}_{i,j}^n - e_{kji}\hat{\omega}_k^n\right)L_j^c = \hat{\gamma}_{ji}^n L_j^c$$

$$\Delta \omega_i^c = F_5\left(\hat{\omega}_{i,j}^n\right) = \hat{\omega}_{i,j}^n L_j^c = \hat{\kappa}_{ji}^n L_j^c$$

- Second-gradient micropolar continuum :

$$\Delta u_i^c = F_6\left(\hat{u}_{i,j}^n, \hat{u}_{i,jk}^n, \hat{u}_{i,jkl}^n, \hat{\omega}_k^n, \hat{\omega}_{k,l}^n \hat{\omega}_{k,lm}^n\right) = \ldots$$

$$\Delta \omega_i^c = F_7\left(\hat{\omega}_{i,j}^n, \hat{\omega}_{i,jk}^n\right) = \ldots$$

Decomposition displacement gradient into symmetric part (strain) and anti-symmetric part :

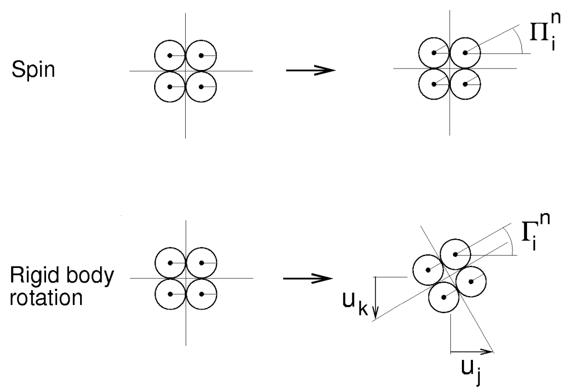
$$\hat{u}_{(i,j)}^n = \hat{u}_{(j,i)}^n = \frac{1}{2}\left(\hat{u}_{i,j}^n + \hat{u}_{j,i}^n\right) = \varepsilon_{ij}$$

$$\hat{u}_{i,j}^n = \hat{u}_{(i,j)}^n + \hat{u}_{[i,j]}^n$$

$$\hat{u}_{[i,j]}^n = -\hat{u}_{[j,i]}^n = \frac{1}{2}\left(\hat{u}_{i,j}^n - \hat{u}_{j,i}^n\right) = -e_{ijk}\hat{\Gamma}_k^n$$

Decomposition of total rotation :

$$\hat{\omega}_i^n = \hat{\Pi}_i^n + \hat{\Gamma}_i^n$$



Definition of stress in terms of contact forces

(Christoffersen *et al.* 1981; Chang, 1988; Bathurst & Rothenburg, 1988; Jenkins, 1988; Chang & Liao, 1990)

- Equilibrium condition:

$$\sigma_{ij,i} = 0$$

- Mean particle stress:

$$\sigma_{ij}^n = \frac{1}{V^n} \int_{V^n} \sigma_{ij} dV = \frac{1}{V^n} \int_{V^n} \left(\sigma_{kj} X_i\right)_{,k} dV$$

- Gauss theorem:

$$\sigma_{ij}^n = \frac{1}{V^n} \int_{S^n} n_k \sigma_{kj} X_i dS$$

- Tractions at particle surface are replaced by sum of contact forces:

$$\int_{S^n} n_k \sigma_{kj} X_i dS = \sum_{c=1}^{N^n} \Sigma f_j^{nc} X_i^n$$

- Local particle stress thus becomes:

$$\sigma_{ij}^{n} = \frac{1}{V^{n}} \sum_{c=1}^{N^{n}} f_{j}^{nc} X_{i}^{n}$$

- Mean volume stress is volume average of local stresses of M particles:

$$\sigma_{ij} = \frac{1}{V} \sum_{n=1}^{M} V^{n} \sigma_{ij}^{n} = \frac{1}{V} \sum_{n=1}^{M} \sum_{c=1}^{N^{n}} f_{j}^{nc} X_{i}^{n}$$

- Branch vector and force equilibrium:

$$L_{i}^{c} = L_{i}^{nm} = X_{i}^{m} - X_{i}^{n} \qquad f_{j}^{c} = f_{j}^{mc} = -f_{j}^{nc}$$

- Two particles *m* and *n* generate one contact:

$$\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N} f_{j}^{c} L_{i}^{c}$$

Constitutive equations for second-gradient micro-polar model

- Stress-force relations:

$$\sigma_{ij} = \frac{1}{V} \sum_{c=1}^{N} f_{j}^{c} L_{i}^{c}$$

$$\mu_{ij} = \frac{1}{V} \sum_{c=1}^{N} m_{j}^{c} L_{i}^{c}$$

- Contact laws:

$$f_{i}^{c} = K_{ij}^{c} \Delta u_{j}^{c}$$

$$m_{i}^{c} = G_{ij}^{c} \Delta \omega_{j}^{c}$$

- Kinematic relations:

$$\Delta u_{i}^{c} = F_{6}\left(\hat{u}_{i,j}^{n}, \hat{u}_{i,jk}^{n}, \hat{u}_{i,jkl}^{n}, \hat{\omega}_{k}^{n}, \hat{\omega}_{k,l}^{n} \hat{\omega}_{k,lm}^{n}\right) = \ldots$$

$$\Delta \omega_{i}^{c} = F_{7}\left(\hat{\omega}_{i,j}^{n}, \hat{\omega}_{i,jk}^{n}\right) = \ldots$$

• Constitutive relations:

$$\sigma_{ij} = A_{ijkl}\varepsilon_{kl} + C_{ijklmn}\varepsilon_{kl,mn} + E_{ijklmn}u_{[k,l]mn} + H_{ijmpq}\Pi_{m,pq} + M_{ijm}\Pi_m$$

$$\mu_{ij} = N_{ijpql}u_{[q,p]l} + R_{ijkl}\Pi_{k,l}$$

• Coefficients are of the form:

$$C_{ijklmn} = \frac{1}{6V}\sum_{c=1}^{N} L_i^c K_{jk}^c L_l^c L_m^c L_n^c$$

$$N_{ijpql} = \frac{1}{2V}\sum_{c=1}^{N} L_i^c G_{jk}^c e_{kpq} L_l^c$$

• Closed-form expressions: isotropic distribution of inter-particle contacts and equi-sized particles

$$\sum_{c=1}^{N} F^c(\gamma,\phi) = \frac{N}{4\pi}\int_0^{2\pi}\int_0^{\pi} F^c(\gamma,\phi)\sin\gamma\ d\gamma\ d\phi$$

Closed-form of second-gradient micro-polar model

$$\sigma_{ij} = \lambda\delta_{ij}\gamma_{kk} + \left(\mu + \frac{1}{2}C_{(3)}\right)\gamma_{ij} + \left(\mu - \frac{1}{2}C_{(3)}\right)\gamma_{ji} + C_{(1)}\delta_{ij}\nabla^2\gamma_{kk} + C_{(2)}\gamma_{kk,ij}$$
$$+ \left(\frac{1}{2}C_{(2)} + \frac{1}{2}C_{(4)}\right)\nabla^2\gamma_{ij} + \left(\frac{1}{2}C_{(2)} - \frac{1}{2}C_{(4)}\right)\nabla^2\gamma_{ji} + C_{(4)}\left(\gamma_{jk,ki} - \gamma_{kj,ki}\right)$$

$$\mu_{ij} = 2C_{(5)}\left(\delta_{ij}\kappa_{kk} + \kappa_{ji}\right) + 2C_{(6)}\kappa_{ij}$$

• Constitutive coefficients are of the form (using $\theta = \frac{Nr^2}{15V}$)

$$\lambda = \theta(4Kn - 4Ks)$$

$$\mu = \theta(4Kn + 6Ks)$$

$$C_{(1)} = \frac{8}{7}\theta r^2(Kn - Ks)$$

$$C_{(2)} = \theta r^2\left(\frac{16}{7}Kn + \frac{12}{7}Ks\right)$$

$$C_{(3)} = 20\theta Ks$$

$$C_{(4)} = 4\theta r^2 Ks$$

$$C_{(5)} = \theta(2Gn - 2Gs)$$

$$C_{(6)} = \theta(2Gn + 8Gs)$$

Reduced forms of the second-gradient micro-polar model

- Linear elastic model, $C_{(1)}$ to $C_{(6)}$ = 0,:

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij}$$

- Second-gradient model, $C_{(3)}$ to $C_{(6)}$ = 0, (Chang & Gao, 1995):

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + C_{(1)}\delta_{ij}\nabla^2\varepsilon_{kk} + C_{(2)}\left(\nabla^2\varepsilon_{ij} + \varepsilon_{kk,ij}\right)$$

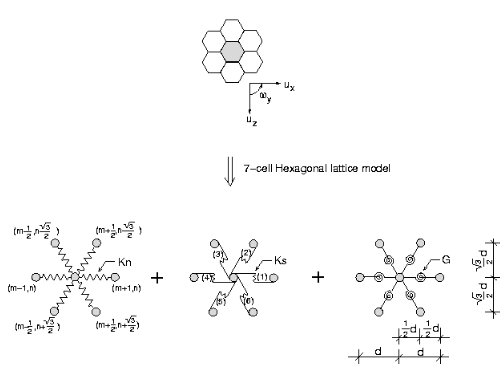
- Cosserat model, $C_{(1)}$, $C_{(2)}$ and $C_{(4)}$ = 0, (Chang & Ma, 1992):

$$\sigma_{ij} = \lambda\delta_{ij}\gamma_{kk} + \left(\mu + \frac{1}{2}C_{(3)}\right)\gamma_{ij} + \left(\mu - \frac{1}{2}C_{(3)}\right)\gamma_{ji}$$

$$\mu_{ij} = 2C_{(5)}\left(\delta_{ij}\kappa_{kk} + \kappa_{ji}\right) + 2C_{(6)}\kappa_{ij}$$

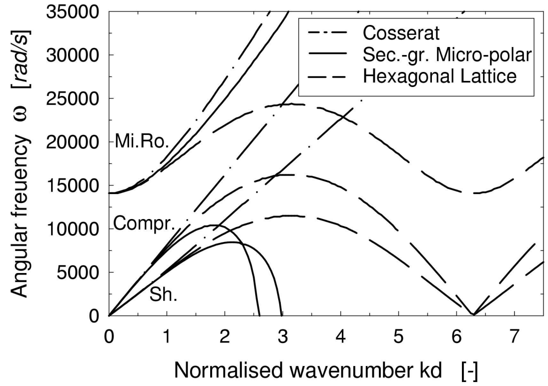
Comparison wave characteristics of continuum models with lattice models

(Suiker, Metrikine & de Borst, 2001)



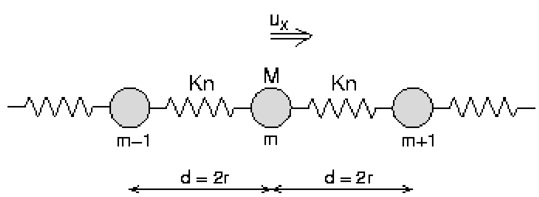
Representation of hexagonal lattice

Dispersion curves for various models



Dispersion curves for compression wave, shear wave and micro-rotational wave

- Discrete Born-Karman lattice model:



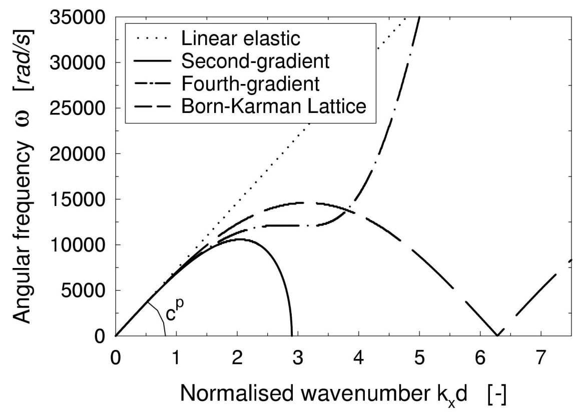
- Second-gradient model:

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + C_{(1)}\delta_{ij}\nabla^2\varepsilon_{kk} + C_{(2)}\left(\nabla^2\varepsilon_{ij} + \varepsilon_{kk,ij}\right)$$

- Fourth-gradient model:

$$\sigma_{ij} = \lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij} + C_{(1)}\delta_{ij}\nabla^2\varepsilon_{kk} + C_{(2)}\left(\nabla^2\varepsilon_{ij} + \varepsilon_{kk,ij}\right) + D_{(1)}\delta_{ij}\nabla^2\nabla^2\varepsilon_{kk}$$
$$+ D_{(2)}\nabla^2\nabla^2\varepsilon_{ij} + D_{(3)}\nabla^2\varepsilon_{kk,ij}$$

Compression wave dispersion curves for various models



Dispersion curves for compression wave

Concluding Remarks

Results presented were taken from:

• A.S..J. Suiker & C.S. Chang (2000), Application of higher-order tensor theory for formulating enhanced continuum models, *Acta Mech.* **142**, pp. 223-234.

• A.S.J. Suiker, R. de Borst & C.S. Chang (2001a), Micro-mechanical modelling of granular material – Part I – Derivation of a second-gradient micro-polar constitutive theory, *Acta Mech.* **149**, pp. 161-180.

• A.S.J. Suiker, R. de Borst & C.S. Chang (2001a), Micro-mechanical modelling of granular material – Part II – Plane wave propagation in infinite media, *Acta Mech*. **149**, pp. 181-200.

•A.S.J. Suiker & R. de Borst (2001), Enhanced continua and discrete lattices for modelling granular assemblies, *Phil. Trans. Roy. Soc. A.* (to appear).