Nonlocal contact evolution and curvature correction in confined granular systems

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MOTIVATION

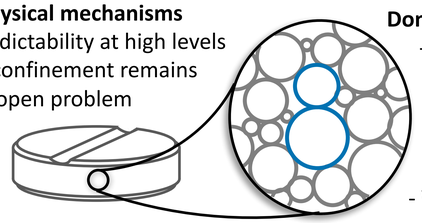
- Powder Compaction is a highly popular manufacturing process and the core of many major industries, especially pharmaceuticals and powder metallurgy.
- Predictive modeling of the macroscopic behavior of confined granular systems is essential for optimizing the process and increasing its efficiency and productivity.

MODELING APPROACH

- **Particle mechanics strategies (models individually describe all particles in the powder bed)**
- Experimentally assisted multi-scale modeling (particle scale models and protocols for characterizing particle properties)

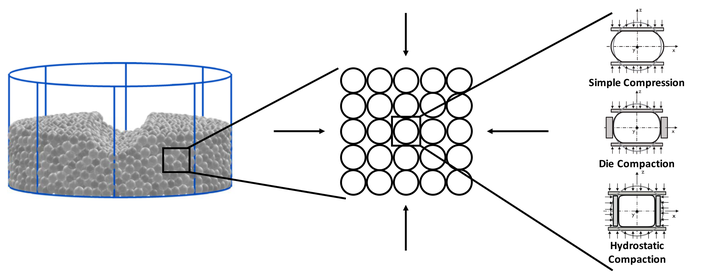
PARTICLE MECHANICS STRATEGIES

- **Predictive constitutive models of inter-particle interactions for a variety of physical mechanisms**
  + Predictability at high levels of confinement remains an open problem



Dominant mechanisms:
- **Elastic deformations**
- **Plastic deformations**
- Bonding
- Strain-rate mechanisms
- Friction and fracture
- Water intake and swelling

- Complex behavior at the granular scale can be simplified by studying three symmetric loading configurations of single particles.



Disordered powder bed | Simplified interpretation for studying single particle behavior | Symmetric loading configurations

- Predictability of particle mechanics approaches relies on the **contact formulation** being employed.

Contact Formulation

- **Elastic**
  - **Hertz Theory (Hertz 1882)**
    - Classical contact mechanics law
    - Assumes independent contacts
    - Applicable to small deformations and low relative densities
  - **Nonlocal Contact Formulation (Gonzalez and Cuitiño 2012)**
    - State-of-the-art contact law
    - Relaxes the assumption of independent contacts by considering deformations due to multiple contact forces on the particle
    - Applicable to moderate deformations and high relative densities
    - Reduces to Hertz theory when nonlocal effects are removed
- **Plastic**
  - **Storåkers Similarity Model (Storåkers 1997)**
    - Contact mechanics law derived using self-similarity approach
    - Assumes independent contacts
    - Applicable to small deformations and low relative densities

THEORETICAL FRAMEWORK (PLASTIC DEFORMATIONS)

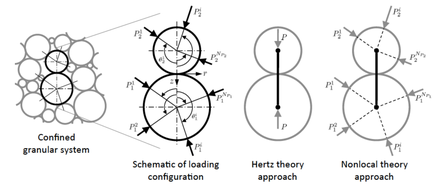


Figure 1: Concept of Nonlocal Theory

- **For elastic particles, formulation is an extension of Hertz Theory**

$$P = \eta_H(\gamma+\gamma_{NL})^{3/2} \quad \eta_H = \frac{4}{3}\left(\frac{1-\nu_1^2}{E_1}+\frac{1-\nu_2^2}{E_2}\right)^{-1}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^{-1/2} \quad \gamma_{NL} = \sum_{k=1,2}\sum_{i=1}^{N_{P_k}} w_{P_k^i}$$

$$w_{P_k^i} \simeq \frac{1+\nu_k}{4\pi R_k E_k}\frac{P_k^i[-2(1-\nu_k)-2(1-2\nu_k)\sin(\theta_k^i/2)+(7-8\nu_k)\sin^2(\theta_k^i/2)]}{\sin(\theta_k^i/2)}$$

- **For plastic particles, formulation could be an extension of Storåkers Law**

$$P = \eta_p(\gamma+\gamma_{NL})^{1+\frac{1}{2m}} \quad \eta_p = 2^{1-\frac{1}{2m}}3^{1-\frac{1}{m}}\pi c^{2+\frac{1}{m}}\kappa_o R^{1-\frac{1}{2m}} \quad \gamma_{NL} = \sum_{k=1,2}\sum_{i=1}^{N_{P_k}} w_{P_k^i}^{pl}$$

$w_{P_k^i}^{pl} = ?$ → **CHALLENGE: PRINCIPLE OF SUPERPOSITION NOT APPLICABLE FOR PLASTIC DEFORMATIONS**

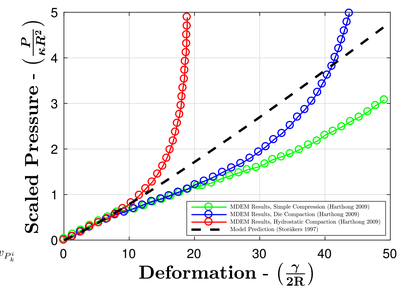


Figure 2: Graph showing the FEM simulation results for plastically deforming lead particles (Harthong 2009), compared with the Similarity solution curve

THEORETICAL FRAMEWORK (ELASTIC DEFORMATIONS)

CURVATURE CORRECTION

Current Formulation:

$$f_1(r) = R_1 - \sqrt{R_1^2 - r^2} \simeq \frac{r^2}{2R_1}, \quad f_2(r) = R_2 - \sqrt{R_2^2 - r^2} \simeq \frac{r^2}{2R_2}$$

which leads to

$$a = \sqrt{(\gamma+\gamma_{NL})\mathbb{A}} \quad P = \frac{4}{3}\left(\frac{1-\nu_1^2}{E_1}+\frac{1-\nu_2^2}{E_2}\right)^{-1}\mathbb{A}^{-1/2}(\gamma+\gamma_{NL})^{3/2}$$

New Formulation:

$$f_1(r) = R_1 - \sqrt{R_1^2 - r^2} \simeq \frac{r^2}{2R_1} + \frac{r^4}{8R_1^3} + \frac{r^6}{16R_1^5} + \frac{5r^8}{128R_1^7} + ...,$$

$$f_2(r) = R_2 - \sqrt{R_2^2 - r^2} \simeq \frac{r^2}{2R_2} + \frac{r^4}{8R_2^3} + \frac{r^6}{16R_2^5} + \frac{5r^8}{128R_2^7} + ...$$

For a 2-term correction, we get

$$a = \left[\frac{3}{2\mathbb{B}}\left(\sqrt{\frac{4\mathbb{B}}{3}(\gamma+\gamma_{NL})+\mathbb{A}^2}-\mathbb{A}\right)\right]^{1/2} \quad P = \frac{4}{3}\left(\frac{1-\nu_1^2}{E_1}+\frac{1-\nu_2^2}{E_2}\right)^{-1}\left[\frac{3}{2\mathbb{B}}\left(\sqrt{\frac{4\mathbb{B}}{3}(\gamma+\gamma_{NL})+\mathbb{A}^2}-\mathbb{A}\right)\right]^{3/2}\left[\mathbb{A}+\frac{3}{5}\left(\sqrt{\frac{4\mathbb{B}}{3}(\gamma+\gamma_{NL})+\mathbb{A}^2}-\mathbb{A}\right)\right]$$

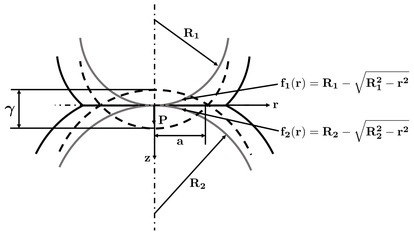


Figure 3: Schematic of the contact between two dissimilar particles

NONLOCAL CONTRIBUTION TO CONTACT RADIUS

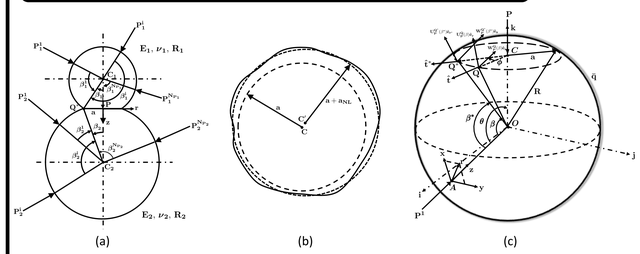


Figure 4: Depiction of nonlocal effects on the contact area between two dissimilar particles being compressed by a general loading configuration. (a). A schematic of the loading configuration (b). The contact configuration without (depicted by a long dashed line) and with (depicted by a solid line) nonlocal evolution. (c). Single loaded boundary value problem depicting a sphere of radius R with an imaginary contact of radius a and contact force P, with concentrated force P^1 acting normally on one of its surface points. Two points Q and Q^* on the contact boundary at an angle ϕ from each other lie at angles β and β^* from the force P^1.

The nonlocal contribution to contact radius, denoted by a_{NL}, is given by

$$a_{NL} \approx \frac{1}{2}\sum_{k=1,2}\left[u_P^{Q^*} + \sum_{i=1}^{N_{P_k}}\frac{1}{2\pi}\int_0^{2\pi} u_{P_k^i}^{Q^*}(\theta_k^i,\phi)d\phi\right]$$

where,

$$u_P^{Q^*} = \frac{(1+\nu_k)P}{4\pi E_k a}\left[\frac{a}{\sqrt{2}R_k}\sqrt{1+\sqrt{1-\left(\frac{a}{R_k}\right)^2}} - 2(1-2\nu_k)\left(1-\frac{1}{\sqrt{2}}\sqrt{1-\sqrt{1-\left(\frac{a}{R_k}\right)^2}}\right)\right]$$

and

$$\frac{1}{2\pi}\int_0^{2\pi} u_{P_k^i}^{Q^*}(\theta_k^i,\phi)d\phi = \frac{1}{2\pi}\int_0^{2\pi}\left[-(W_{P^1}^{Q^*} - W_{P^1}^{C})\sin\theta\cos\phi + (U_{P^1}^{Q^*} - U_{P^1}^{C})\sqrt{1-\sin^2\theta\cos^2\phi}\right]d\phi$$

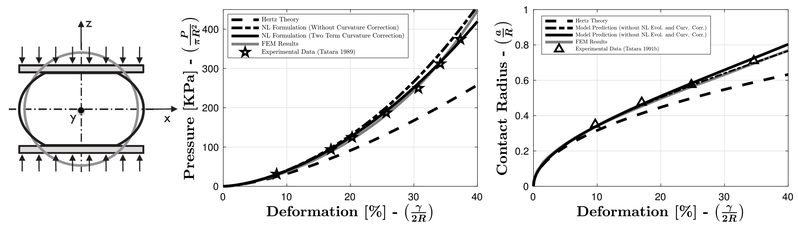
$$\simeq \frac{(1+\nu_k)P_k^i}{16\pi R_k E_k}\left(\frac{a}{R_k}\right)\frac{\cos^2\left(\frac{\theta_k^i}{2}\right)}{\sin\left(\frac{\theta_k^i}{2}\right)}\left[4\nu - 3 - \cos\theta_k^i + \left(\frac{a}{R_k}\right)^2\frac{-57+(28+5\cos\theta_k^i-36\nu_k)\cos\theta_k^i+60\nu_k}{64\sin^2\left(\frac{\theta_k^i}{2}\right)}\right]\left(1-\frac{\theta_k^i}{\pi}\right)$$

$$+\frac{(1+\nu_k)P_k^i}{4\pi E_k a}\left[\frac{a}{\sqrt{2}R_k}\sqrt{1-\sqrt{1-\left(\frac{a}{R_k}\right)^2}} - 2(1-2\nu_k)\left(1-\frac{1}{\sqrt{2}}\sqrt{1+\sqrt{1-\left(\frac{a}{R_k}\right)^2}}\right)\right]\left(\frac{\theta_k^i}{\pi}\right)$$

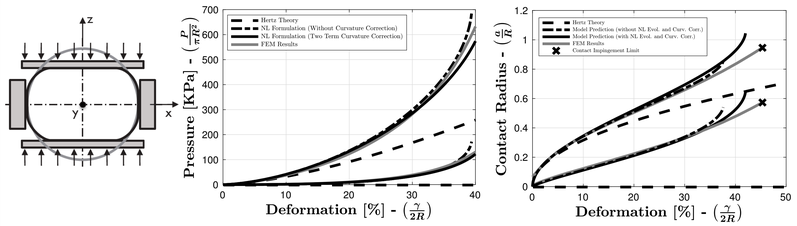
SIMULATION RESULTS

- Simulations were performed for spherical rubber particles with E = 1.85 MPa, ν = 0.48 and R = 10 mm.

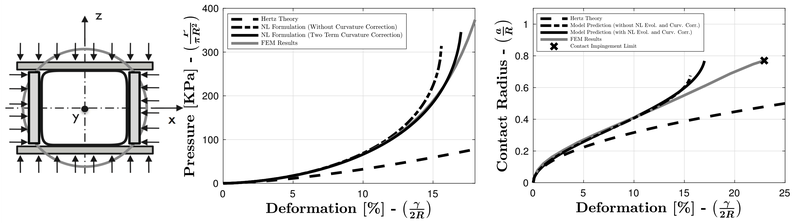
SIMPLE COMPRESSION



DIE COMPACTION



HYDROSTATIC COMPACTION



CONCLUSIONS AND FUTUTRE WORK

- A new, improved version of the nonlocal contact formulation for elastic particles was developed by introducing curvature correction and nonlocal contact evolution.
- Good agreement was obtained between the predictions of finite-element model and nonlocal contact formulation for evolution of force and contact area with deformation. Nonlocal contribution to contact radius and curvature correction were found to improve the prediction of contact impingement.
- Extension of nonlocal formulation to finite plastic deformations remains a topic of future research.

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