Compaction rheology of soft granular materials

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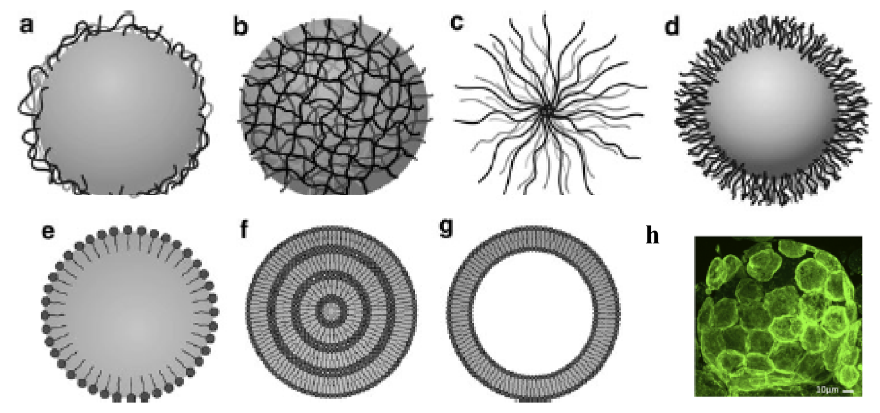
JMC 17 — Journées de la Matière Condensée, du 24 au 27 Août 2021

Context

Granular materials are an important class of matters found in the nature and in a large number of industrial fields like civil engineering, food and pharmaceutical industries, powder technologies (chemistry, cosmetics...), etc. In many situations, these materials can be highly stressed and their constitutive particles undergo large deformations without rupture. It means that the behavior of soft granular systems is governed by both interactions between particles (contact, adhesion...) and their individual behavior (elasticity, plasticity…). They can reach packing fractions beyond Random Close Packing (RCP) state and they flow by both particle shape change and collective rearrangements.

We investigate the texture and rheology of ultrasoft granular systems by means of numerical simulations using the Material Point Method (MPM) to model particle deformability, combined with the Contact Dynamics (CD) method for the treatment of contacts between particles [1-4].



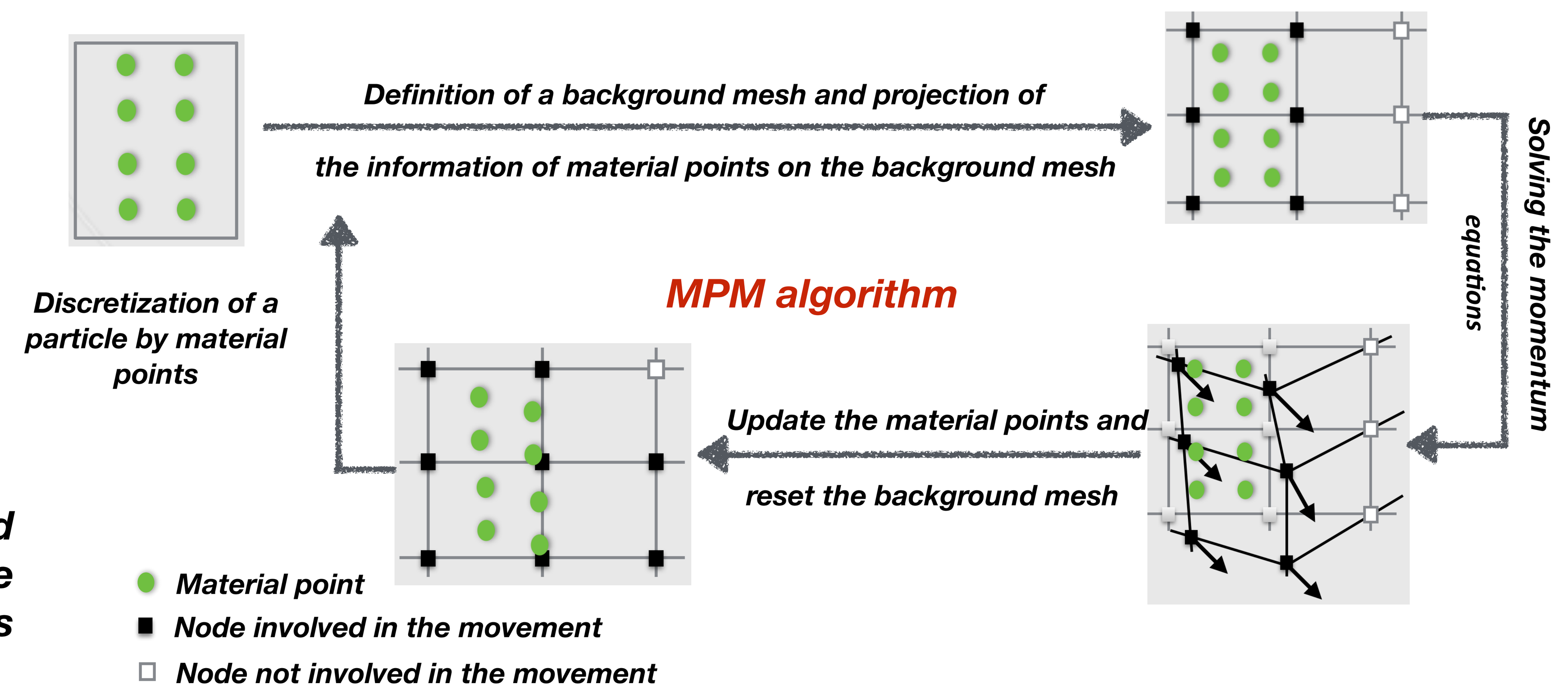
Various types of soft particles: (a) solid particle covered with adsorbed or grafted polymer chains; (b) microgel particle; (c) star polymer; (d) block copolymer micelle; (e) emulsion droplet; (f) multi-lamellar vesicle; (g) liposome; (h) biological cell (according to Bonnecaze and Cloitre, Apl. Poly. Sci. 2010).

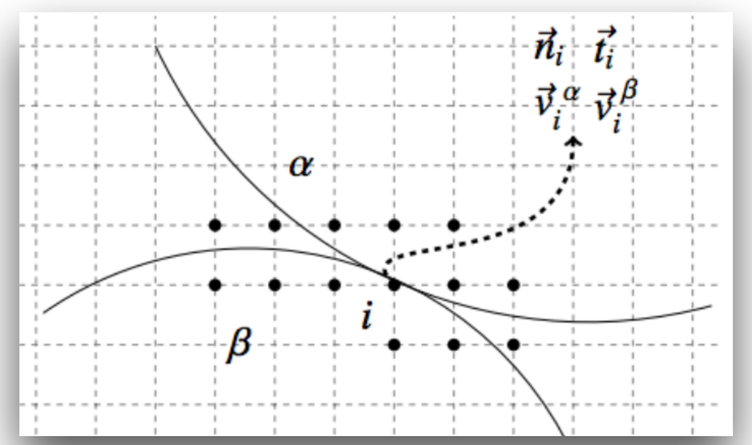
Numerical methodology

Material Point Method (MPM)

The MPM is a finite element method with mobile integration points. Each particle is discretized by a set of material points with fixed masses carrying all state variables such as stress and velocity field. The MPM algorithm also uses a background mesh for solving the momentum equations.

Our technique for modeling of soft-article materials is based on interfacing the MPM, for dealing with the bulk behavior of particles, with the CD method for the treatment of frictional contacts.





A multi-mesh contact algorithm is used to implement contact laws such as the friction Coulomb law or adhesion laws at the contact points.

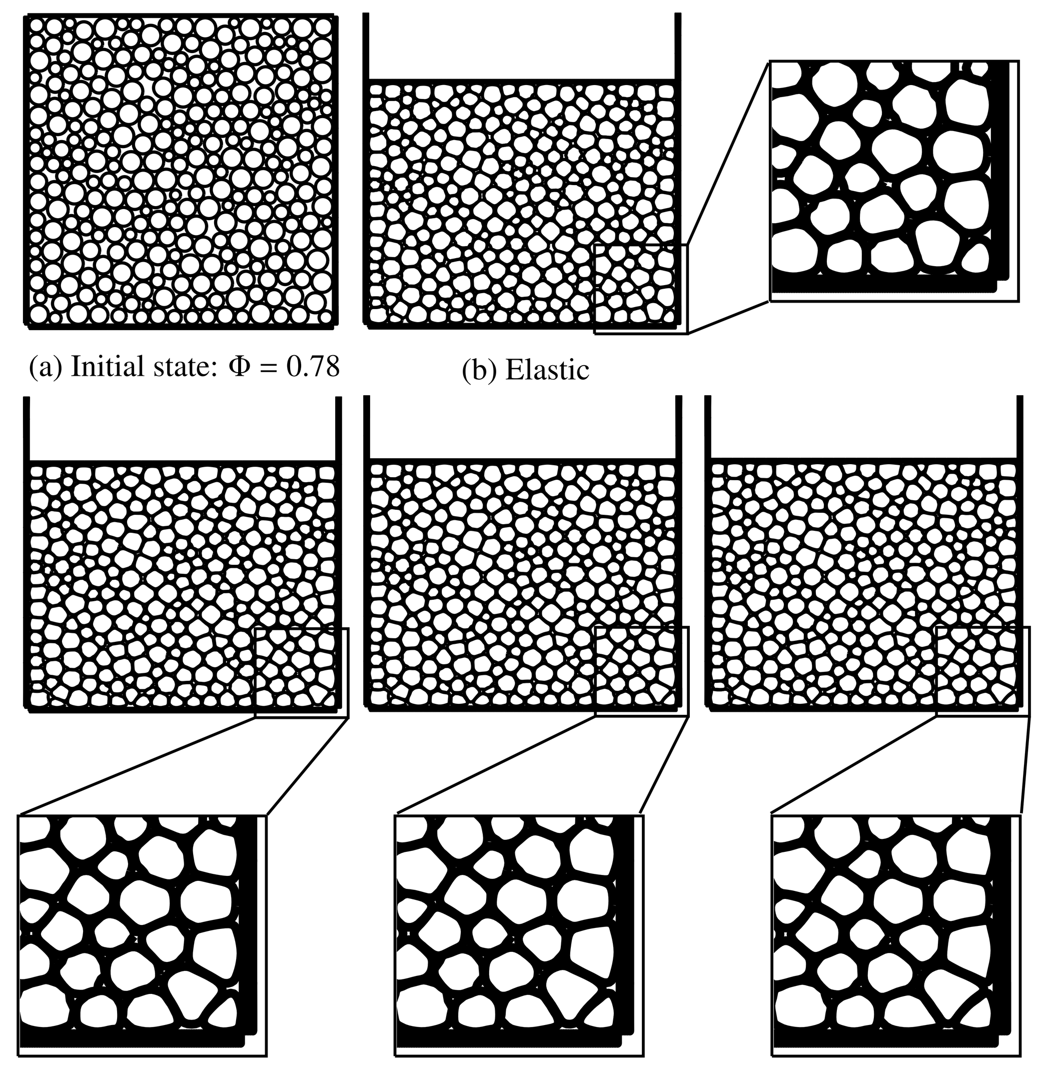
Uniaxial compression of an assembly of soft particles

Uniaxial compaction of 300 deformable particles particles confined in a rigid box is carried out using MPM simulations. The initial configuration is prepared by means of CD simulations. A small size polydispersity is introduced in order to avoid long-range ordering. The coefficient of friction between the particles, and between the particles and the walls is set to zero.

Material properties : *Elasto-plastic constative law with linear isotropic hardening*

$\rho = 1000\ Kg/m^3$, $E = 10\ MPa$, $\nu = 0.45$, $\sigma_y = 0.4\ MPa$ and $H = 0,\ 1,\ 3\ MPa$

A snapshot of initial configuration and the snapshots of the packing for $\Phi \simeq 0.97$



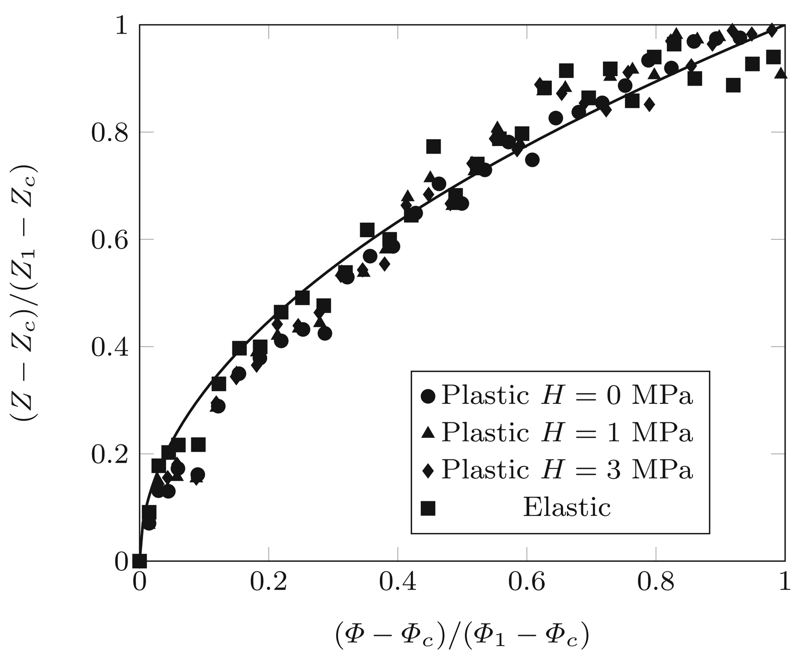
(a) Initial state: $\Phi = 0.78$ (b) Elastic (c) Plastic H=3 MPa (d) Plastic H=1 MPa (e) Plastic H=0 MPa

Evolution of average coordination number Z as a function of packing fraction Φ

This power law relation fits the data points:

$$\frac{Z - Z_c}{Z_1 - Z_c} = \left(\frac{\Phi - \Phi_c}{\Phi_1 - \Phi_c}\right)^{0.5}$$

Here, Z_c and Φ_c correspond to the jamming point, and Z_1 and Φ_1 correspond to a dense state that can be reached for a confinement stress that tends towards infinity. This relation is almost independent of dimension, interaction potential or polydispersity (O'Hern et al. PRE 2003). In the above relation, there is no adjusting parameter.



Theoretical description above the jamming point [4]

The vertical stress σ as a function of the packing fraction Φ for the elastic particles can be expressed as follows:

$$\sigma = -\frac{1}{\frac{1}{M^{eff}} + \frac{1}{c_1 Z \Phi}}(\ln(\Phi) + c_2)$$

Granular materials like a porous media —> $M^{eff} = \dfrac{\mu^{eff}(4\mu^{eff} - E^{eff})}{3\mu^{eff} - E^{eff}}$ *with* $E^{eff} = E\left(1 - \dfrac{p}{p_c}\right)^{f_E}$ *and* $\mu^{eff} = \mu\left(1 - \dfrac{p}{p_c}\right)^{f_\mu}$.

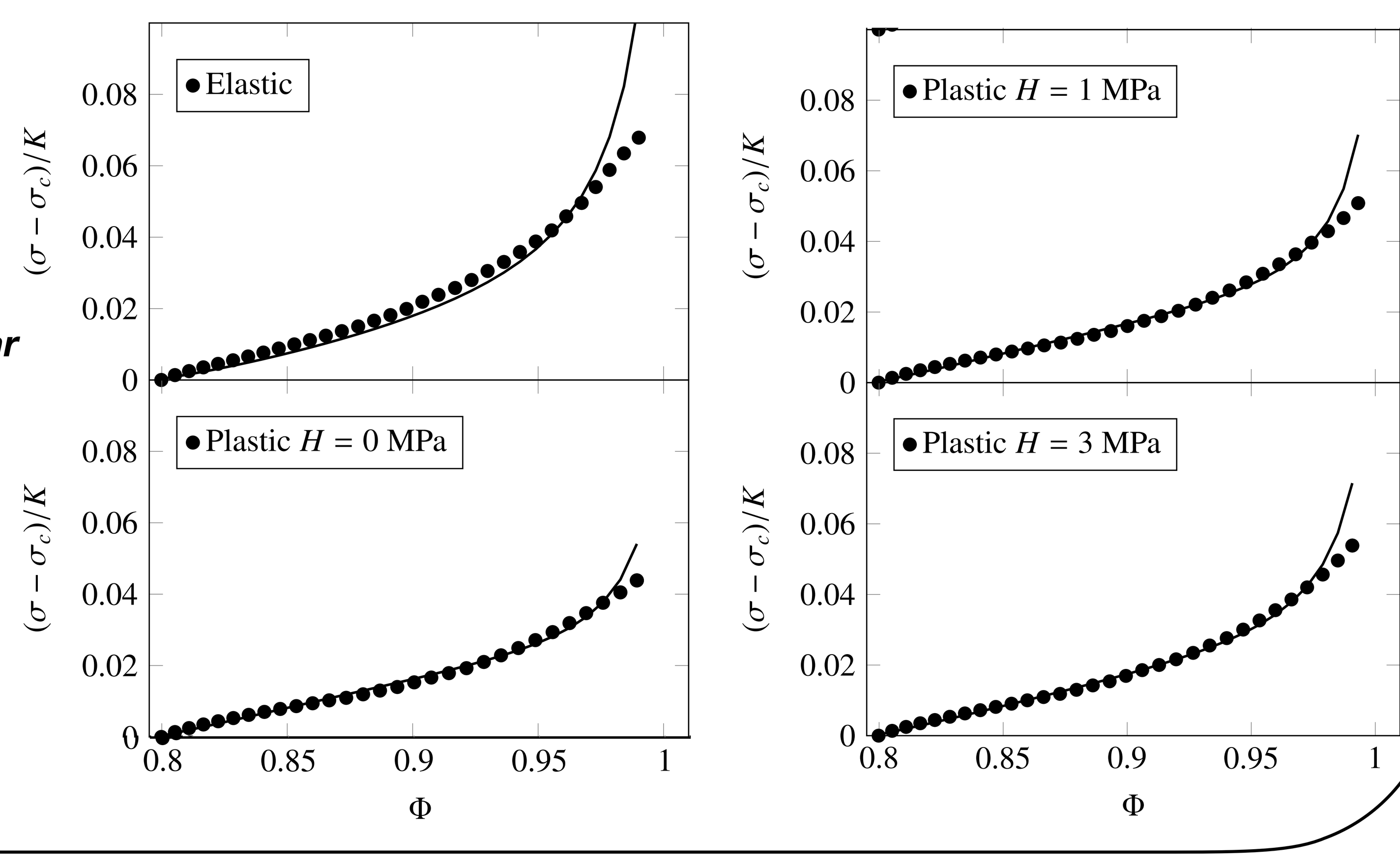
Here, p is the porosity ($p = 1 - \Phi$), f^E and f^G denote the characteristic components for Young's and shear moduli, and p_c is the critical porosity, below which the effective Young's and shear moduli become zero.

For the plastic particles: the stress is decomposed into an elastic part σ_e and a plastic part σ_p:

$\sigma = (1 - f_p)\sigma_e + f_p \sigma_p$ *with f_p as the plastic volume fraction* ($f_p = \alpha \ln\left(\dfrac{\Phi}{\Phi_c}\right)$).

This model can predict the behavior of the assembly of elasto-plastic particles with:

$$c_1 = 100,\ p_c = 0.201(\simeq 1 - \Phi_c),\ f_E = 1.1,\ f_\mu = 0.1,\ c_2 = 0.23(\simeq -\ln(\Phi_c))\ \&\ \alpha = 2.5$$



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