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ScienceDirect

Procedia Engineering 175 (2017) 141 – 147

Procedia Engineering

www.elsevier.com/locate/procedia

1st International Conference on the Material Point Method, MPM 2017

# MPM with frictional contact for application to soft particulate materials

Saeid Nezamabadi[a,*], Thanh H. Nguyen[a,c], Jean-Yves Delenne[b], Julien Averseng[a], Xavier Frank[b], Farhang Radjai[a,d]

[a] *Laboratoire de Mécanique et Génie Civil (LMGC), Université de Montpellier, CNRS, Montpellier, France*
[b] *Ingénierie des Agro-polymères et Technologies Émergentes (IATE), UMR1208, INRA, Université de Montpellier, Cirad, SupAgro, Montpellier, France*
[c] *Water Resources Engineering Department, Da Nang University of Technology, Da Nang University, 54 Nguyen Luong Bang St, LienChieu Dist, Da Nang, Vietnam*
[d] *<MSE>[2] , UMI 3466 CNRS-MIT, CEE, Massachusetts Institute of Technology (MIT), 77 Massachusetts Avenue, Cambridge CA 02139, USA*

**Abstract**

Soft particle materials are composed of discrete particles that can undergo large deformations without rupture. Most food products, many powders, colloidal pastes, vesicles and biological cells are soft particle systems. In order to model such materials, we present an efficient numerical approach combining an implicit formulation of the Material Point Method (MPM) and Contact Dynamics (CD) method. The MPM deals with bulk variables of an individual particle by discretizing it as a collection of material points, whereas the CD allows for the treatment of frictional contacts between particles. This model is applied for the simulation of the uniaxial compression of 2D soft-particle packings. The compaction is a nonlinear process in which new contacts are formed between particles and the contact areas increase. The change of particle shapes allows these materials to reach high packing fraction. We find that the contact specific surface, the orientation anisotropy and the aspect ratio of particles increase as a function of the packing fraction but at different rates. We also evidence the effect of friction, which favors strong stress chains and thus the elongation of particles, leading to larger values of the orientation anisotropy and the aspect ratio at a given level of packing fraction as compared to a frictionless particle packing.



Peer-review under responsibility of the organizing committee of the 1st International Conference on the Material Point Method

*Keywords:* material point method; contact dynamics; soft matter; granular materials.

## 1. Introduction

Soft particles are the main component of many natural and industrials materials like colloidal pastes, microgels, suspensions, etc. In these materials, there is a disordered discrete network of soft particles which governs their behaviors by a combination of particle rearrangements and particle shape change. So, the properties of soft particle materials depend on both theirs discrete natures (contact interactions, rearrangements...) and their particle continuum

* Corresponding author.
*E-mail address:* saeid.nezamabadi@umontpellier.fr

1877-7058 
Peer-review under responsibility of the organizing committee of the 1st International Conference on the Material Point Method
doi:10.1016/j.proeng.2017.01.044

behaviors (deformability, compressibility...). Indeed, these particles can undergo large deformation without rupture. All of these features allow these materials to achieve high packing fractions beyond Random Close Packing (RCP) state. Because of these complexities of soft particle systems, many aspects of their behaviors and properties under compression and shear should be until explored.

Particular materials are mainly simulated using numerical strategies based on Discrete Element Methods (DEM). In the DEM, these materials are modeled as a collection of undeformable particles and the elastic deformations may be assumed at the contact points. The most common discrete methods based on hard particles are Molecular Dynamics (MD) [1] and Contact Dynamics (CD) [2,3]. Although the DEM techniques are known as mature and efficient approaches to model and analyze particular materials, they are intrinsically unable to account for realistic constitutive models of individual particles and large particle deformations. So, in order to deal with both continuum and discrete behaviors of soft particle materials, it is necessary to introduce the internal degrees of freedom for each individual particule as well as to treat contact interaction between different particles.

A promising numerical procedure has been developed to investigate a packing of soft particles in our previous papers [4,5]. This approach combines two numerical tools: it uses first an implicit formulation of Material Point Method (MPM) [6] to take into account the constitutive continuum behaviors of particles. In this approach, each particle is discretized by a collection of material points. The information carried by the material points is projected onto a background mesh, where equations of motion are solved. The mesh solution is then used to update the material points. The second tool which is related to the contact treatment, is based on the Contact Dynamics. The CD method is a general approach for the treatment of frictional contacts without regularization. It was pioneered by a mathematical formulation of non-smooth mechanics by Moreau [7] and then extensively used for the simulation of granular materials with rigid grains [8,9]. This method is based on an implicit time-stepping scheme and formulated in terms of grain velocities, which may undergo jumps as a result of collisions and non-smooth feature of the Coulomb friction law. Since we use an implicit MPM scheme, the CD method is a natural choice for the treatment of contact points. The implicit MPM-CD formulation was implemented in a manner that the contact variables can be computed simultaneously with bulk variables. In this paper, we apply this MPM algorithm to analyze the compaction of a packing of soft particles. We investigate the respective roles of rearrangements, particle volume change and particle shape change to compaction by analyzing different rheological parameters (packing fraction and, contact specific surface, orientation anisotropy and aspect ratio of particles).

## 2. Material point method (MPM)

Let us consider a continuum body occupying a domain $\Omega$ in $\mathbb{R}^D$, $D$ being the domain dimension. In the context of the infinitesimal strain theory, its conservations of mass and of linear momentum can be described by the following relations:

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} + \boldsymbol{\nabla} \cdot (\rho(\mathbf{x},t)\, \mathbf{v}(\mathbf{x},t)) = 0 \quad \text{in } \Omega\,, \tag{1}$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) = \rho(\mathbf{x},t)\, \mathbf{a}(\mathbf{x},t) \quad \text{in } \Omega\,, \tag{2}$$

where $\rho(\mathbf{x},t)$ is the material density, $\boldsymbol{\sigma}(\mathbf{x},t)$ denotes the Cauchy stress tensor, $\mathbf{b}(\mathbf{x},t)$ represents the body force and, $\mathbf{v}(\mathbf{x},t)$ and $\mathbf{a}(\mathbf{x},t)$ are the velocity and the acceleration, respectively, at position $\mathbf{x}$ and time $t$. A constitutive relationship should supplement the continuity equation (1) and momentum equation (2). We assume here a linear, homogeneous, isotropic and elastic relationship:

$$\boldsymbol{\sigma}(\mathbf{x},t) = \mathbb{C} : \boldsymbol{\epsilon}(\mathbf{x},t)\,, \tag{3}$$

where $\mathbb{C}$ refers to fourth-order elastic tensor and $\boldsymbol{\epsilon}$ denotes the strain tensor ($\boldsymbol{\epsilon} = \frac{1}{2}(\boldsymbol{\nabla}\mathbf{u} +^t \boldsymbol{\nabla}\mathbf{u})$; $\mathbf{u}$ being the displacement field). Note that, in this formulation, any other material behavior (including inelastic behaviors) may be implemented.

In the MPM, the continuum body is divided into $N_p$ material points with constant masses. This last assumption allows satisfying automatically the mass conservation relation (1). The material points represent the integration points