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The legacy of Jean-Jacques Moreau in mechanics

Multi-periodic boundary conditions and the Contact Dynamics method

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ABSTRACT

For investigating the mechanical behavior of granular materials by means of the discrete element approach, it is desirable to be able to simulate representative volume elements with macroscopically homogeneous deformations. This can be achieved by means of fully periodic boundary conditions such that stresses or displacements can be applied in all space directions. We present a general framework for periodic boundary conditions in granular materials and its implementation more specifically in the Contact Dynamics method.

1. Introduction

Granular materials are of primary importance in a variety of scientific and technological areas such as soil mechanics, geological processes and flows, soft matter physics, powder technology and agronomy. Frictional-contact interactions between particles and physical and/or chemical effects of an interstitial fluid or solid material lead to a nonlinear rheological behavior that has not yet been fully formulated in the framework of a continuum theory. In particular, the state variables in quasi-static and/or inertial granular flows and their evolution with shear strain reflect the complex evolution of the contact network, and still need to be clearly identified and included in a continuum description of the plastic behavior.

The particle-scale variables have been a subject of constant experimental investigation for fifty years, and many features pertaining to the contact network such as fabric anisotropy and force distributions have been analyzed. This move towards particle-scale modeling was later reinforced by the application of the Discrete Element Method (DEM) for the simulation of particle dynamics [1–12]. The DEM is based on the step-wise integration of the equations of motion for all particles, described as rigid elements, by accounting for contact interactions and boundary conditions. The DEM can also be seen as an application of the Molecular Dynamics (MD) method to rigid particles. The perfectly rigid nature of the particles involves only the rigid-body degrees of freedom, but the application of classical explicit integration methods requires a regular (smooth) *force law* at the contact point between two particles with a *contact deflection* defined from their overlap. Generally, the repulsive force is considered to be proportional to the overlap and a viscous damping term is added to account for inelastic collisions.

A new approach to the DEM emerged from a mathematical formulation of nonsmooth dynamics and algorithmic developments by J.-J. Moreau and M. Jean [13–21]. This approach, called Contact Dynamics (CD), is based on a nonsmooth

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formulation of particle dynamics in the sense that the particle velocities and contact forces are simultaneously computed at each time step from the balance of momenta by taking into account the unilateral contact interactions and Coulomb friction law, hence without introducing contact deflection and a repulsive potential. The CD method has been applied to investigate granular materials [22–29,9,30–33], as well as masonry and tensegrity structures [34,35]. For static and plastic shear properties, the CD simulations agree well with MD simulations [36,22,37–40]. The main difference between the two methods in their application to granular materials is the resolution of elastic time scales in the MD method in contrast to the CD method, in which the natural time unit is imposed by particle dynamics and external actions [37,9,41].

The application of the DEM for the investigation of the rheology of granular materials is hindered by the relatively low number of numerically tractable particles as compared to that in real materials. In most reported DEM simulations both in 2D and 3D, the number of particles is below 10^4, as a result of the restrictions imposed by available computation power and memory. As a consequence, the numerical samples are not always statistically representative of the bulk behavior but are also influenced by spurious wall effects. The packing fraction is generally lower in the vicinity of rigid walls and wall-induced ordering can deeply propagate into the bulk. The distortion of a confining walls can also lead to arching at the corners and generate stress gradients over long distances inside the numerical sample [42]. Such effects are real and arise also naturally in experiments on granular materials. However, the number of particles in experiments is generally much higher and hence the wall effects are more critical in numerical simulations.

The undesired effects of wall-like boundaries can be removed by means of periodic boundary conditions. The simulation domain under periodic conditions becomes a unit cell containing the particles with periodic replica of the cell and its particles paving the whole space. Hence, the particles belonging to the borders of the cell interact only with other particles inside the cell or with their images in the neighboring image cells; see Fig. 4. As a result, the periodic conditions extend the system boundaries to the infinity and the simulation cell simply plays the role of a coordinate system locating particle positions [43]. In other words, the origin of the coordinates becomes immaterial so that the resulting dynamics is invariant by translation and therefore necessarily homogeneous.

In this paper, we present a detailed description of the formulation of periodic boundary conditions for the CD method. Such an extension of the method to periodic boundaries is not theoretically straightforward as it involves periodicity not only in particles positions but also in nonaffine particle velocities and in equations of dynamics. A consistent and general formulation should allow for the application of either stresses or displacements in all directions of space. To do so, the role of the walls should be replaced by the collective degrees of freedom carried by the coordinate system. In this way, the basis vectors become dynamic variables, and their conjugate stresses are expressed as a state function of the granular configuration. This method was first introduced by Parrinello and Rahman for a Hamiltonian conservative system [44]. We extend this approach to granular materials, which are not generally conservative systems as a result of frictional and collisional inelastic dissipation.

In the following, we first introduce the CD method. Then, we consider in detail the kinematics, equations of dynamics and time-stepping schemes under periodic boundary conditions. Finally, we show how the equations of contact dynamics should be modified under periodic boundary conditions. We conclude with a few remarks about the implementation.

2. Contact Dynamics method

2.1. Contact laws

Consider two particles i and j touching at a contact point κ inside a granular material. We assume that a unique common line (here in 2D) tangent to the two particles at κ can be defined. The contact can therefore be endowed with a local reference frame defined by a unit vector $\vec{n}$ normal to the line and a unit vector $\vec{t}$ along the line. A potential (or prospective) contact exists if the gap δ_n between two particles (partners) is sufficiently small so that a collision may occur between the two particles within a small time interval δt (time step in numerical simulations). If the contact is effective ($\delta_n = 0$), a repulsive (positive) normal force f_n may appear at κ with a value depending on the particle velocities and forces exerted on the two partners by their neighboring particles; see Fig. 1. But if $\delta_n > 0$ (nonzero gap), the contact is not effective and f_n is identically zero. These conditions can also be by the "complementarity relations" $\delta_n \geq 0$, $f_n \geq 0$ and $\delta_n f_n = 0$ or cast into the following Signorini's inequalities:

$$\begin{cases} \delta_n > 0 & \Rightarrow \quad f_n = 0 \\ \delta_n = 0 & \Rightarrow \quad f_n \geq 0 \end{cases} \tag{1}$$

Obviously, this relation can not be reduced to a (mono-valued) functional dependence between δ_n and f_n.

The above conditions imply that the normal force vanishes when the contact is not effective. However, the normal force may also vanish at an effective contact. This is the case for $u_n = \dot{\delta}_n > 0$, i.e. for incipient opening of a contact. Otherwise, the effective contact is *persistent*, and we have $u_n = \dot{\delta}_n = 0$. Hence, Signorini's inequalities can be extended as follows:

$$\begin{cases} \delta_n > 0 \Rightarrow f_n = 0 \\ \delta_n = 0 \ \wedge \ \begin{cases} u_n > 0 & \Rightarrow \quad f_n = 0 \\ u_n = 0 & \Rightarrow \quad f_n \geq 0 \end{cases} \end{cases} \tag{2}$$