Moment transfer law in a three dimensional spherical discrete element model : theoretical developments

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ABSTRACT

A discrete element method with spherical elements is used to study the behaviour of geomaterials. Previous simulations have shown the limitation of this elements' geometry to reproduce accurately the shearing behaviour, because of its rolling overstate compare to real granular, imposed to add to the local constitutive law with a contact moment. Once this local enrichment formulation added, the model should be able to reproduce accurately the bending and torsion behaviour modes of simple beams. Finally, the aim of this new development is to improve the ability of spherical discrete elements to reproduce generalized behaviours of geomaterials. Therefore, different methods for controlling the rotational behaviour in rolling or torsion mode are presented and compared to this formulation. Another advantage of this local constitutive law, compared to the classical spherical DEM, is to keep a low calculation cost.

INTRODUCTION

Circular or spherical discrete elements ([1], [2] and [3a, 3b]) are widely used to simulate geomaterial behaviours. The behaviour law's characterization study depends on the problem's scale. The simulation range can be from full structures to small volumes of material. Because of the rotational invariance of spherical elements the numerical implementation of the contact detection algorithm is simpler to apply than for polyhedral and ellipsoidal elements and the time required for computation is lower. The main drawback of using spherical elements is that excessive rolling occurs during a shear displacement [4]. Such models underestimate the value of the friction angle as compared to real geomaterials. While keeping the simplicity of the spherical geometry of elements, it is possible to act upon this rolling by preventing the rotations of elements ([5], [6]). In biaxial simulations, only sliding will then occur, which in

turn, will result in a better value of the friction angle [2]. However, this extreme option gives good results for axial loading, however for shear loading, the rolling process can not be ignored [7]. A moment transfer can be added to the local constitutive law of DEM to keep the advantages of the spherical geometry. Let's call this MTL "Moment Transfer Law" for further reference. By adding this MTL, the rolling which occurs during shear displacement is decreased, and a better value of the friction angle is reached. This modification of the constitutive law was first created for two dimensional assemblies of disks representing purely frictional material such as sand ([8], [9]), and named "Modified distinct element model" -MDEM -. It was created in order to have a rolling resistance in a DEM model of granular materials. As the scale of the problem can range from a rock sample to a structure, other types of materials should be involved and thus modelled. Here, this moment transfer has been developed for three dimensional problems. It seems that purely frictional and cohesive granular materials, as well as other classical materials used in civil engineering such as steel can be modelled by introducing this MTL within the DEM. For example, a single line of discrete elements is needed to represent the bending behaviour of an elastic beam by using MTL, when several parallel lines were necessary with classical DEM. The MTL can be completed by introducing a torsion component. By including elastic limits in bending and torsion for spherical discrete elements, a more realistic model of materials might be obtained.

JUSTIFICATION AND DESCRIPTION OF THE MTL

Numerical model

In order to do the numerical study, the software SDEC [3a, 3b] has been used. The constitutive laws that govern the behaviour of the simulated geomaterials can be described by the following points:

1. Discrete elements are non-deformable and homogeneous-like spheres.

2. Interactions between elements follow a force – displacement method, as used by Cundall [1]).

3. Discrete elements in interactions can slightly overlap at the contact point and the mathematical relation between normal or shear force and normal or tangential displacements are linear.

4. The yield of an interaction during a local shear process follows the Mohr-Coulomb criterion. Tension strength with softening can also be used.

A detailed description of the constitutive laws can be found in [3a]. The classical discrete element method does not prevent the rotation of elements that are assumed to have free rotations governed by tangential forces acting at the contact point on each element.

Representativeness of a shear process with spherical discrete elements

The advantage of using spherical elements is that the detection of contacts, as well as the inertial description, is fast and simple. However, this simple geometry limits the mechanical possibilities of the model. During a shear process, rolling takes place at the local scale and is controlled by the angularity and roughness in granular materials. The spherical elements enhance this rolling phenomenon thus leading to lower values of shear resistance. By increasing the local friction angle, the global friction angle is more significant, and reaches a limit value ([2], [4], [6]) around 25° for three-dimensional assemblies [10]. As the friction angle of geomaterials easily reaches a value of 35° , it seems difficult to simulate granular material correctly. It is also possible to restrain the rotation of elements partially [5] or totally [2], and thus limit rolling of elements. This aspect can be used to simulate biaxial or triaxial

tests on granular materials ([2], [5]), and also at the structure scale ([6], [11]). When rolling is completely removed, only sliding can take place during a shear displacement. The simulated friction angle can reach values corresponding to those of geomaterials. In this case the value of the global friction angle is higher than the local one [2] and the post-rupture softening that can be observed during real tests is low [9]. Simulation tests have shown that the rolling process is two times more significant than sliding process in the shear band for circular and elliptic elements [2]. Experimental results are equivalent [7]. Thus rolling phenomenon is not intrinsic to spherical geometry and is necessary to describe a shear process correctly. An intermediate method has been built up ([10], [12]). Rotation and rolling are allowed but can be controlled by an artificial moment which is opposite to the direction of rolling. This is what is done in MDEM and it gives a qualitatively correct dense granular material behaviour during biaxial tests on a collection of disks [12]. The relation between axial and volumetric deformations is more realistic than when the rotations are either free or blocked. Softening and shear bands can be identified as in real cases. However, with this method the rolling resistance that governs the quantitative aspects of the shear process must be calibrated to match the values of the simulated granular material.

Description of the MTL

The formulation of the two dimensional MDEM is now extended to three dimensional cases for spherical elements, and is input into the SDEC software. In order to be able to reproduce the torsion phenomenon also, the constitutive laws of the classical DEM were also modified along the axis of two elements in interaction. This formulation is presented in a second part.

Rolling resistance using the MTL

The rolling phenomenon depends on the relative rotation of two spheres. The following equations are expressed in a global reference G in order to integrate the modifications caused by the MTL, into the constitutive laws. Let two spheres A and B, be in contact (Figure 1). The radiuses of these spherical elements are r_A and r_B . In the global reference, their positions are defined by two vectors \vec{x}_A and \vec{x}_B , while their rotations are given by $\vec{\omega}_A$ and $\vec{\omega}_B$. Their rotation velocities are $\vec{\omega}_A$ and $\vec{\omega}_B$ and incremental rotation occurring during the timestep are given by



Figure 1: Evolution of the contact between spheres A and B for two time steps t and t+dt

 $\overrightarrow{d\omega_A}$ and $\overrightarrow{d\omega_B}$. The normal vector to the contact occurring at the point C, is defined by \vec{n} , and is directed from element A to element B. Considering two successive simulation times, the new positions of the centres A' and B' are defined by the vectors $\vec{x_A}$ and $\vec{x_B}$. The new contact point is now C', when the new normal to the contact is $\vec{n'}$. A mean radius r can be defined where,

$$r = \frac{r_A + r_B}{2} \tag{1}$$

The rolling part of an interaction between two spheres can be described when the incremental rotation and the sliding components are identified. Let C_A and C_B be defined by the following equations:

$$\overrightarrow{A'C_A} = \overrightarrow{AC}$$
(2)

$$B'C_B = \overrightarrow{BC}$$
(3)

The vectors $\overrightarrow{C'C_A}$ and $\overrightarrow{C'C_B}$ are both linked to the translation motion and to the sliding process of each sphere:

$$\overline{C'C_A} = r_A(n-n') \tag{4}$$

$$\overrightarrow{C'C_B} = r_B(\overrightarrow{n'} - \overrightarrow{n}) \tag{5}$$

The material point of element A (or B) which is located at point C at time t is found at point M_A (or M_B) at time t+dt. The following vectors can be defined:

$$\overrightarrow{C_A M_A} = r_A \cdot dt \, \overrightarrow{\omega_A} \wedge \overrightarrow{n} \tag{6}$$

$$\overrightarrow{C_B M_B} = -r_B dt \overrightarrow{\dot{\omega}_B} \wedge \overrightarrow{n}$$
(7)

The relative positions of M_A and M_B , compared to the new contact point C' correspond to the sum of both the translation and pure rotation vectors:

$$\overrightarrow{C'M}_{A} = \overrightarrow{C'C}_{A} + \overrightarrow{C}_{A}\overrightarrow{M}_{A} = r_{A}((\overrightarrow{n} - \overrightarrow{n'}) + dt\overrightarrow{\dot{\omega}}_{A} \wedge \overrightarrow{n})$$
(8)

$$\overrightarrow{C'M}_{B} = \overrightarrow{C'C}_{B} + \overrightarrow{C}_{B}\overrightarrow{M}_{B} = r_{B}((\overrightarrow{n'} - \overrightarrow{n}) + dt\overrightarrow{\omega}_{B} \wedge \overrightarrow{n})$$
(9)

It is temporarily assumed that the two spheres have identical radiuses. By doing so, the expressions for sliding, rolling and pure rotation are easy to write. The incremental displacement vector $\overrightarrow{dU_r}$, caused by the rolling process is given by:

$$\overrightarrow{dU_r} = \frac{\overrightarrow{C'M_A} + \overrightarrow{C'M_B}}{2}$$
(10)

By studying two particular cases the link between vector $\overline{dU_r}$ and the rolling process can be better understood. First consider that the two spheres undergo a pure sliding process. The components of the incremental rotations defined in Eq.6 and Eq.7 are equal to zero and because of the opposite signs in Eq.4 and Eq.5, Eq. 10 vanishes.

In the second case, let the relative sliding be zero and let the spheres have an opposite rotation velocity. The normal to the contact is unchanged after a time step, thus Eq.4 and Eq.5 vanish. The incremental rotations given in Eq.6 and Eq.7 are equal, allowing Eq.10 to be different from zero. It is then a pure rolling process.

To represent geomaterials, assemblies of elements are not built up with spheres of the same radius. Supposing that the scale ratio is not too important, then the Equation (10) can be also used in order to define the rolling part. An equivalent expression was used in the 2D case in the disk assembly [10]. The rolling process corresponds to a rotation and is defined by the angular rolling vector $\overline{d\theta_r}$. The action – reaction principle suggests that an identical value of moment should be applied on both spheres in contact. Its value is defined by the mean value acting at the interaction point. The unitary vector $\overrightarrow{n_{d\theta_r}}$ oriented along $\overrightarrow{d\theta_r}$ is defined by:

$$\overrightarrow{n_{d\theta r}} = \frac{\overrightarrow{n'} \wedge \overrightarrow{dU_r}}{\left\| \overrightarrow{n'} \wedge \overrightarrow{dU_r} \right\|}$$
(11)

The angular vector of incremental rolling is given by:

$$\overrightarrow{d\theta_r} = \frac{\left\| \overrightarrow{dU_r} \right\|}{r} \overrightarrow{n_{d\theta r}}$$
(12)

Let the vector $\overrightarrow{\theta_r}$ be defined by the addition of the angular vectors of incremental rolling since the contact creation between the two observed elements:

$$\vec{\theta}_r = \sum \vec{d\theta_r}$$
(13)

The constitutive law associated to the MTL is created in order to reproduce both elastic and plastic behaviours. A limit value of the moment modulus needs to be implemented in order to be able to reproduce these behaviours. If this value is reached, the moment creates irreversible deformations. To establish if the plastic limit has been reached, the rolling angle is defined in a local set of axes *L*. The centre of *L* is at point *C*, and its axes are the normal vector \vec{n} , and two perpendicular vectors $\vec{t_1}$, $\vec{t_2}$ which are in the contact plane.

Let θ_r^L , the angular vector of the rolling part in the set of axes L, be given by

$$\overrightarrow{\theta_r^L} = \left[m_{G_{-L}} \right] \overrightarrow{\theta_r}$$
(14)

Where $[m_{G_{-L}}]$ defines the transition matrix from the global set of axes G to the local one L. Only the components acting into the contact plane have to be considered to define the rolling resistance, because the first component is directed along the normal to the contact \vec{n} . Its value must be set to zero. Let k_r be the rolling stiffness. If an isotropic rolling behaviour is assumed, this value is a scalar. The elastic moment \overline{M}_{elast}^L created by the rolling part in L is written as:

$$\overline{M_{elast}^{L}} = k_r \overline{\theta_r^{L}}$$
(15)

Let η be a dimensionless parameter of the elastic limit of rolling, which controls the elastic limit of the rolling behaviour. If $\|\overrightarrow{F_n}\|$ represents the norm of the normal force at the contact

point, and *r* is the mean value of the two radiuses, the elastic limit is given by the plastic moment vector \overline{M}_{plast}^{L} such that:

$$\overrightarrow{M_{plast}^{L}} = \eta r \left\| \overrightarrow{F_{n}} \right\|$$
(16)

The applied moment corresponds to the minimal norm of the two moments defined by Eq.15 and Eq.16, directed along the vector defined by Eq.12. Let $[m_{L_G}]$ be the transition matrix from the local reference *L* to the global reference *G*, then the rolling moment $\overrightarrow{M_r}$ is given by:

$$\overline{M_{r}} = \overline{m_{L_{G}}} \min\left(\left\|\overline{M_{elast}}^{L}\right\|, \left\|\overline{M_{plast}}^{L}\right\|\right) \frac{M_{elast}^{L}}{\left\|\overline{M_{elast}}^{L}\right\|}$$
(17)

The value $-\overrightarrow{M_r}$ is then applied on element *A*, while the opposite value is exerted on element *B*, according to the action – reaction principle. Finally, if the elastic limit is reached at the current timestep, then the angular rolling vector $\overrightarrow{\theta_r}$ has to be modified in order to take into account the effect of irreversibility. Its value has to be modified before being written into the global reference for later iterations.

$$\overrightarrow{\theta_r^L} = \frac{M_{plast}^L}{k_r}$$
(18)

To summarize, the MTL is given by the following system of equations:

If
$$\left\| \overrightarrow{M_{elast}^{L}} \right\| < \left\| \overrightarrow{M_{plast}^{L}} \right\|$$
: $\overrightarrow{M_{r}} = \begin{bmatrix} m_{L_{-}G} \end{bmatrix} \overrightarrow{M_{elast}^{L}}$ and $\overrightarrow{\theta_{r}^{L}} = \frac{M_{elast}^{L}}{k_{r}}$
(19)
If $\left\| \overrightarrow{M_{elast}^{L}} \right\| \ge \left\| \overrightarrow{M_{plast}^{L}} \right\|$: $\overrightarrow{M_{r}} = \begin{bmatrix} m_{L_{-}G} \end{bmatrix} \overrightarrow{M_{plast}^{L}} \frac{\overrightarrow{M_{elast}^{L}}}{\left\| \overrightarrow{M_{elast}^{L}} \right\|}$ and $\overrightarrow{\theta_{r}^{L}} = \frac{\overrightarrow{M_{plast}^{L}}}{k_{r}}$ (20)

Model of a torque transfer with the MTL

For a structure such as a cylindrical beam, the torsion phenomenon corresponds to a section rotation around the neutral axis. The torsion moment is given by the torsion stiffness modulus and the unit angular variation. When modelling this beam with a single line of discrete elements, a similar behaviour is obtained. Let's start again with the configuration given in Figure 1. $\overrightarrow{\omega_A}$ and $\overrightarrow{\omega_B}$ are the rotational vector of the elements in the global set of axes *G*. the relative rotational vector between elements *A* and *B* is given by :

$$\overrightarrow{\omega_{rel}} = \overrightarrow{\omega_A} - \overrightarrow{\omega_B}$$
(21)

This relative rotational vector is written in the local set of axes L by using the transition matrix $[m_{G_{-L}}]$:

$$\overrightarrow{\omega_{rel}^{L}} = \left[m_{G_{L}}\right] \overrightarrow{\omega_{rel}}$$
(22)

The relative rotation $\overrightarrow{\omega_{rel}^L}$ is expressed in the set of $\operatorname{axes}(\vec{n}, \vec{t_1}, \vec{t_2})$. Unlike the rolling moment case, the component along \vec{n} only has to be considered. The torsion moment has to be applied at the interaction point. If we consider that the two elements have the same size, a linear interpolation of the relative rotation at the interaction point $\overrightarrow{\omega_M}$ is given by:

$$\overrightarrow{\omega_M} = \frac{1}{2} \overrightarrow{\omega_{rel}^L}$$
(23)

This value is correct for two spheres with identical radiuses, and is acceptable as long as the spheres are close in size. Let k_i define the torsion stiffness modulus. The elastic moment in

torsion $\overline{T_{elast}^{L}}$ can be written in the local set of axes as,

$$\overrightarrow{T_{elast}^L} = k_t \overrightarrow{\omega_M}$$
(24)

It is also possible to create an elastoplastic model for the torsion behaviour, by considering a limit value $\overrightarrow{T_{plast}^{L}}$ for the elastic moment norm. In the global set of axes *G*, the moment $\overrightarrow{T_{t}}$ to apply on both elements is given by:

$$\vec{T}_{t} = \left[m_{L_{G}}\right] \min\left(\left\|\vec{T}_{elast}^{L}\right\|), \left\|\vec{T}_{plast}^{L}\right\|\right) \frac{T_{elast}^{L}}{\left\|\vec{T}_{elast}^{L}\right\|}$$
(25)

The value $-\overrightarrow{T_t}$ is applied on element *A* while the opposite value is applied on element *B*. If the interaction is in a plastic state, the angular rotation vector $\overrightarrow{\omega_{rel}}$ has to be modified, in order to take into account the effect of irreversibility. In this case, its local expression is modified according to the following equation, before being later expressed in the global reference system,

$$\overrightarrow{\omega_{rel}^L} = \frac{\overrightarrow{T_{plast}^L}}{k_t}$$
(26)

To summarize, the MTL used to account for torsion is given by the following system of equations:

If
$$\left\| \overline{T_{elast}^L} \right\| < \left\| \overline{T_{plast}^L} \right\|$$
: $\overline{T_t} = \left[m_{L_G} \right] \overline{T_{elast}^L}$ and $\overline{\omega_{rel}^L} = \frac{\overline{T_{elast}^L}}{k_t}$ (27)

If
$$\left\| \overrightarrow{T_{elast}^L} \right\| \ge \left\| \overrightarrow{T_{plast}^L} \right\|$$
: $\overrightarrow{T_t} = \left[m_{L_a} \right] \overrightarrow{T_{plast}^L}$ and $\overrightarrow{\omega_{rel}^L} = \frac{T_{plast}^L}{k_t}$ (28)

Behaviours associated to k_r and k_t

Use of the k_r stiffness for a granular material

The MTL can be used for granular materials in order to generate a resistant moment that is opposite to the rolling behaviour. This should compensate for the drawbacks associated to the use of spherical shaped elements. The rolling stiffness parameter k_r defines the level of

influence that the resistant moment produces, depending on Eq.15. Let $\overrightarrow{dU_r}$ and $\overrightarrow{dU_s}$ be the incremental vector of the rolling and sliding parts. The two-dimensional formula [9], is extended into 3D to obtain the following equation:

$$\overline{dU_r} \cong \overline{dU_s} \tag{29}$$

When the sliding and rolling process are considered, if k_s represent the shear stiffness of the interaction and *r* is the mean radius of the two spheres, the following equation for the 3D case is obtained:

$$k_{s}\overrightarrow{U_{s}}\times \overrightarrow{rn} \cong k_{r}\frac{\overrightarrow{dU_{r}}}{r}\times \overrightarrow{n}$$
(30)

The expression for k_r in the 2D case is [9]:

$$k_r = k_s r^2 \tag{31}$$

This expression is acceptable for unequal sphere sizes if the ratio between the smallest and the biggest element is low [9]. Rather than using the mean value as in Eq.31, the relative size of both spheres could be used. Real granular materials are angular which limits the rolling process. If two grains are very different in size, the shape of the biggest is almost locally a plane as seen by the smallest element. Then the rolling process may be considered as controlled by the smallest element. The radius parameter to be used in Eq.31 is then given by:

$$r = \min(r_A, r_B) \tag{32}$$

For elements which have about the same size, this last expression is approximately equivalent to the one given by Eq.1. It thus has an influence mainly when the elements have different sizes.

Use of k_r to represent the bending moment acting on a beam

The MTL formulation can also be used to simulate the quasi-static behaviour of beams. In the system of axes R, defined by $\vec{n_x}, \vec{n_y}, \vec{n_z}$, consider a cylindrical beam oriented along the $\vec{n_x}$ unit vector. The radius of this cylinder is R. Suppose this beam has an isotropic behaviour, its Young's modulus is E and its quadratic moment is I, which is constant along each direction of the cross section. When external forces act on the beam, the corresponding bending moment is given by the following differential equation:

$$\frac{d\omega_i}{dx} = \frac{M_i}{EI}$$
(33)

 ω_i corresponds to the angular variation of the neutral axis, relative to the initial state without forces acting on the beam. The MTL can be used to generate a moment at each interaction point, which corresponds to the bending moment that is observed in real materials and that classical DEM can not represent. Eq.33 can be discretized in order to be inserted in the constitutive law. According to Figure 1, the angular vector $\vec{\omega}$ corresponds to a relative rotation $\vec{\theta_r}$ between the two spheres, while dx can be associated to the sum of the two radiuses of the elements. The quadratic moment I_f is invariant in any direction perpendicular to the beam axis and can be expressed by:

$$I_f = \frac{R^4 \pi}{4} \tag{34}$$

Finally, the numerical expression of the bending moment, acting at the interaction point can be written:

$$\overrightarrow{M} = \frac{EI_f}{r} \overrightarrow{\theta_r}$$
(35)

This model can simulate the behaviour of a beam in a bending mode by using a single line of identical discrete elements. However, this can also be used for elements of unequal size. In this case, the following formulation of the quadratic moment, using Eq.1 and Eq.34, has to be preferred:

$$I_f = \frac{r^4 \pi}{4} \tag{36}$$

$$\overrightarrow{M} = \frac{EI_f}{r} \overrightarrow{\theta_r}$$
(37)

The stiffness k_r is defined by Eq.15 and Eq.37:

$$k_r = \frac{EI_f}{r} \tag{38}$$

Use of k_t to represent the torsion moment acting on a beam

The beam defined in 2.4.2, has a bulk modulus G and a quadratic moment I_t when in torsion mode. ω_M is supposed to define one half of the relative angular rotation between the two spheres, according to Eq.23. Depending on the mechanical properties, as was done in Eq.34 and Eq.35, the quadratic moment around the neutral axis and the elastic moment produced by the torque can be written:

$$I_{t} = \frac{\pi R^{4}}{2}$$

$$\overrightarrow{M} = \frac{2GI_{t}}{R} \overrightarrow{\omega_{M}}$$
(39)
(40)

The stiffness given by Eq.24 and Eq.40 is:

$$k_t = \frac{2GI_t}{R} \tag{41}$$

A limit value for the torsion elastic behaviour is also put into the model to generate irreversibility. Using the same idea as in the bending phenomenon (see 2.4.2), the torsion behaviour simulated by the last equations can be extended to assemblies of unequal sphere sizes. This can be done by approximating the radius R, used to define Eq.39 and Eq. 40 with the value of the radius r, defined in Eq.1.

Use of k_t to represent a torsion resistance in granular materials

The bending part of the MTL can be used to exert a resistant moment to the rolling phenomenon. As done previously to control bending, the relative rotation of the two spheres around a common axis may be controlled. This can be done by introducing a resistant moment, opposed to this rotation. This increases the shear capacity of the simulated media while the classical DEM is unable to. The elastic behaviour is equivalent to the one describe in 2.4.3 with Eq.40. In order to obtain a complete Coulomb like behaviour, this moment has an elastic limit value. Here again, the resulting elasto-plastic behaviour is able to reproduce irreversibility. If the local friction angle ϕ and the local tangential cohesion c, which both act on the contact are considered, let r_{\min} be the smaller radius of the two spheres and let F_n be the

norm of the normal force of the contact. Let F_n act uniformly on the contact region of the two spheres. This region is defined as a circular area with a radius r_{\min} . The elastic limit of this torsion moment M, given by the Mohr-Coulomb criterion, is written:

$$M = \frac{2}{3} (r_{\min} F_n \tan \phi + \pi r_{\min}^3 c)$$
(42)

CONCLUSION

In order to limit the rolling phenomenon, the constitutive laws of a spherical discrete element code have been modified. The resulting model is known as MTL. The theoretical basis of this model for bending and torsion have been given. Furthermore boundary values for the elastic couples generated during bending or torsion have been taken into account, in order to reproduce a plastic behaviour. When using the MTL, the real behaviour of materials should be approached quantitatively more so than with classical DEM, but with low cost than any model not using spherical elements. The torsion law can be used for simple beam problems, but can also be considered as a new parameter that can be introduced in simulations of granular materials. This model has been used for almost one year, and simulations results of loaded beams, but also of triaxial tests on granular materials will be further presented.

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