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Continuum modelling of the granular flows in gaseous states using material point method

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ABSTRACT

In a quick flow of granular material, the initially densely packed material often starts to separate and its behaviour changes to that characteristic of a liquid and, at low enough density, to the state where grains are disconnected from the other grains (gaseous states). Modelling such a flow requires acknowledging the changes in the granular material, in particular noting the changes in the constitutive behaviour as well as having the capability to model large displacements and deformations. This study employs the Material Point Method to model the behaviour of granular material flow in transition from the solid to the gaseous state and from the gaseous to the solid state. The paper introduces modifications into the method to represent the changes in the granular material and the constitutive behaviour required for modelling of the granular material in the disconnected regime. This is the first step in application of the Material Point Method in modelling of the flow behaviour of granular material through its various states.

KEY WORDS: granular flow; computational method; material point method

Introduction

Granular flow leads to a very significant amount of shear deformations to granular material, which causes qualitative change in the material behaviour. The granular material are, generally, not capable of supporting tension. However, before initiation of flow, a static body of grains can sustain relatively high shear stress before a substantial initial shear deformation occurs. This early behaviour results in a combination of small reversible and irreversible (elastic and plastic) strains, volumetric and shear stresses and reduce shearing resistance of granular body significantly. After this initial small strain behaviour, the rate of strain increases and the body of soil starts entering flow-like regime. This leads to a sizeable shear deformations, as well as the simultaneous increase of volumetric strains. These shear and volumetric strains are combinations of both elastic and plastic strains, where the elastic part is more significant initially, but while the shearing continues the plastic part becomes dominant. This increase of deformations continues, up to a critical point where in the grains of the material loose constant frictional contacts with their neighbours. At this point, the behaviour of material may enter the flow / gas regime, with the rate of flow becoming the deciding factor. If the flow rate is in more moderate range, volume change is relatively small, material remains in critical state and the stress state is dependent on the shear rate (Kamrin, 2010a; Kamrin and Bazant, 2007; Redaelli et al., 2016). An example of such flow behaviour is flows that happen in an hour glass. On the other hand, high flow rate leads granular grains to lose frictional contacts, become disconnected, interact mainly through collisions and go through very fast deformations and density reduction (Dunatunga and Kamrin, 2015; Redaelli et al., 2016). This paper refers to such state as gaseous state.

Continuum modelling of granular flow through these described stages is challenging. Behaviour of flowing material changes significantly when grains become disconnected and this change is not limited to stress state. Up to now, few researches have used Material Point Method (MPM) for continuum modelling of granular flow (Dunatunga and Kamrin, 2015, 2017; Redaelli et al., 2017). These contributions model the disconnected state by defining a constitutive model based on the kinetic theory, switching the stress behaviour when a certain volume related state is reached and assuming that using a proper constitutive model would prevent disconnected particles from interaction with others. The studies did not investigate the effects of constitutive model on MPM algorithm and whether a mere change of constitutive model would allow for a replication of disconnected states. Furthermore, more advanced versions of MPM face problems when applied to modelling of the disconnected state of flow (Dunatunga and Kamrin, 2017), which prevents their use, even though they are more capable of modelling shear deformations and thus more suitable for modelling other stages of granular flow.

This paper proposes a solution for modelling disconnected granular flow, which is viable for all versions of MPM. It examines advantages and disadvantages of different solutions for modelling disconnected granular and introduces a method that improves...
the shortcoming of previous solutions. The discussion in the following is limited to 1D formulation and the 2D and 3D generalised formulations will be investigated in the future.

**Constitutive model**

The behaviour of granular flows changes significantly in different stages of flow thus a combination of constitutive models and switching mechanisms are required to model the stages of the flow. After a granular material reaches the critical state (defined as no change of volumetric strain upon shearing), its behaviour depends on the specific volume. If the specific volume of the granular material (or a related parameter like void ratio) remains below the critical value, then flow is in moderate range. Otherwise, the flowing material becomes disconnected and in collisional regime (Dunatunga and Kamrin, 2015; Redaelli et al., 2016). The stress state of moderate flow depends to critical state behaviour – for example Kamrin and Bazant (2007) and Kamrin (2010b) consider a rate dependent critical state stress behaviour and describe it with a Bagnold scaling rheology. On the other hand, Redaelli et al. (2016) assumes no dependency between the critical state stress and the rate of flow. Comparing results of Seyedan and Słowski (2017) and Ceccato and Simonini (2016) in estimation of granular flow impact force in small scale experiments shows that the rate dependant critical state stress replicates moderate granular flow quite more accurately. In order to estimate stress state during a disconnected flow, Redaelli et al. (2016) uses kinetic theory of granular gases to predict the collisional stress in a granular flow. This study shows that the collisional stress is low unless the deformation rate is extremely large. Similarly, Dunatunga and Kamrin (2015) and Dunatunga and Kamrin (2017) use the kinetic theory to derive an equation of state for a granular flow. This equation of state approximates a disconnected flow as a stress free state.

In this research, we use the stress free approximation of Dunatunga and Kamrin (2015, 2017), who assumed that when the density of a flowing material dips below a critical value, it indicates transition into a disconnected behaviour. In this disconnected state, the stress is due to a contribution of collisional behaviour of the grains. This contribution is very small unless the deformation rate of flow is extremely high. These extremely fast flows are not the focus of this study. Therefore, we neglect the collisional contribution to the stress state and assume that there is zero stress in the flowing material in the disconnected state. Such a stress-free modelling of the disconnected state of flow requires changes in the Material Point Method implementation and will be discussed in the next section.

**Material point method**

This section investigates modelling the disconnected state of flow with different formulations of the Material Point Method. In the disconnected state, the grains lose frictional contacts and cannot change velocity and position of other grains except via collisions. However, as we assume zero stress, we disregard the collisions of the particles. The zero stress also means that the material points should not interact with each other during the simulation. Previous research, e.g. Dunatunga and Kamrin (2015, 2017) and Redaelli et al. (2017), which used MPM for modelling disconnected state, did not investigate capabilities of different MPM formulations with respect to the modelling of the disconnected state. This section examines these capabilities, compares different solutions for modelling the disconnected stage and suggests a method to improve shortcomings of the previously proposed approaches.

The Material Point Method is primarily used for simulation of problems with very large deformations. Sulsksy et al. (1994) first introduced MPM for continuum mechanic problems. This original method approximates the solid continuum with material points and employs a background grid for calculations, such that it ensures conservation of momentum. Newer formulations of MPM, (e.g. Bardenhagen and Kober, 2004a; Sadeghirad et al., 2011, 2013) differs mainly in how they transfer the data from the material points to the grid and back. The original MPM defines material points merely as points with mass, velocity, stress and internal variables. Furthermore, it uses a linear tent basis function and its gradient to transfer the point data to grid, which allows for the points interaction. The original MPM algorithm employs the same functions to update the material point data afterwards. Subsequently, the Generalized Interpolation Material Point Method (GIMP) by Bardenhagen and Kober (2004b) introduced particle characteristic function, which define the space occupied by a material point. The particle characteristic function is usually a top hat function, leading to a non-overlapping material point domains. Furthermore, GIMP method also employs a formulation which use linear tent function and its gradient to transferring the data between the material points and the grid. Two commonly used variants of GIMP are uGIMP and cpGIMP. The uGIMP assumes that the particle domain is constant. On the other hand, cpGIMP tracks variations of particle domains while assuming that the particle domain remains rectangular. Building on cpGIMP, the Convected Particle Domain Interpolation (CPDI) by Sadeghirad et al (2013) updates the formulation, so that CPDI can track the variations of particle domain size and shape (allowing for shear deformation in particle domain).

These different ways of transferring data and choice of functions leads to material points contributing to different numbers of grid cells during the calculations. In the original MPM formulation (Sulsksy et al., 1994), given material point contributes only to nodes of the grid cell it currently is. However, in uGIMP, material points can also contribute to nodes of some neighbouring grid cells. Nevertheless, the domain of a material point does not change in uGIMP, which limits the number of grid cells and grid cell nodes a material point can contribute to. In the cpGIMP and CPDI formulations, the particle domain size change. This allows material points to contribute to an increasing number of nodes.
Figure 1 shows an initial state for a 1D material, which we will use to examine how different MPM formulations can simulate the disconnected state. In Figure 1, material point 1 is in the gaseous state while all the other points are in the solid state. Material point 1 velocity \( \mathbf{v}_1 \) is in an opposite direction to the velocity of other particles \( \mathbf{v}_2, \mathbf{v}_3 \) and velocity of particles differ in size \(|v_1| \neq |v_2| \neq |v_3| \neq |v_4|\). Furthermore, there are no external forces, tractions and boundary conditions (see Figure 1).

![1D example of particle disconnection](image)

In the original MPM formulation, material point 1 and 2 are the only points contributing to the grid node 3. Following the MPM algorithm, the mass \( m_3 \), momentum \( p_3 \) and the internal force \( f_{3 int} \) of node 3 are:

\[
\begin{align*}
m_3 &= N_1 m_1 + N_2 m_2 \\
p_3 &= N_1 p_1 v_1 + N_2 p_2 v_2 \\
f_{3 int} &= -dN_1 \rho_1 v_1^2 + dN_2 \rho_2 v_2^2
\end{align*}
\]

where \( m_3, p_3 \) and \( f_{3 int} \) are mass, momentum and internal force of node 3, \( N_1, N_2, dN_1, dN_2 \) are the shape functions and their gradients for material point 1 and 2, respectively, and \( m_1, m_2, p_1, p_2, v_1, v_2, \rho_1, \rho_2 \) are mass, velocity, volume and stress of points 1 and 2, respectively. Equation 1 and 2 show that nodal mass and nodal momentum are not affected either by the particle stress nor the constitutive model. Also, both points 1 and 2 contribute to the values of nodal mass and nodal momentum and the node internal force. Therefore, even a stress free approximation of disconnected state \( (\sigma = 0) \) would not result in force free node \( (f_{3 int} = 0) \). After the calculation of these nodal values, the momentum of node 3 is updated:

\[
p_3 = p_3 + f_{3 int} \, dt
\]

where \( dt \) is the calculation time step. The updated nodal momentum allows to update the velocity and the position of the material points, and in particular the material point 1:

\[
\begin{align*}
v_1 &= v_1 + \left( \frac{f_{3 int}}{m_3} N_1 + \frac{f_{3 int}}{m_2} N_2 \right) \, dt \\
x_1 &= x_1 + \left( \frac{p_3}{m_3} N_1 + \frac{p_2}{m_2} N_2 \right) \, dt
\end{align*}
\]

where \( x_1 \) is position of particle 1. \( m_2, p_2 \) and \( f_{2 int} \) are mass, momentum and internal force of node 2. In equation 5 and 6, values of \( m_2, p_2 \) and \( f_{2 int} \) are affected by the velocity, volume and stress of material point 2. Therefore, the assumption that a suitable choice of constitutive model for the disconnected particle (particle 1) prevents it from interaction with other particles is incorrect.

As the material point domains do not change in the original MPM, the material points 1 and 2 in Figure 1 will stop interacting after one of the particles moves to another grid cell and the points will have no longer a common grid node to which they both contribute. Even though the particle domain do not change in uGIMP, material points may contribute to the nodes of the neighbouring grid cells as well as to the cell the material point is currently in. Hence, the material point 3 in Figure 1 may also participate in node 3 calculation, which further connects material point 1 to the material points 2 and 3. Furthermore, material points 1 and 2 will not stop interacting immediately after one of them moves to another cell but will keep interacting as long as they have a common node to which they contribute to. Ultimately, these particles will move further away, contribute to no common node, stop interacting, and the disconnection will happen. Finally, in cpGIMP and CPDI formulations, the domains of particles change and the material points can contribute to an increasing number of nodes. Therefore, points 1 and 2 in Figure 1 will keep interacting and never fully disconnect. Such a behaviour is not correct for the gaseous state of the material.

The solution of the above problem requires introduction of a discontinuity into the method. The proposed algorithm for the disconnected flow is inspired by the work of Nairn (2003), who proposed a method, suitable for any MPM formulation, for modelling explicit cracks in MPM. The Nairn (2003) algorithm allows for displacement and velocity discontinuities. That is achieved as the material points on the same side of a crack share the same velocity field and interact with each other, while the material points on the opposite side of the crack does not. The proposed scheme for modelling of disconnected state suggests similar solution: the material points that interact with each other contribute to the same velocity field, while each disconnected
particle (in a gaseous state) has its own velocity field. Particle velocity fields merge after the material points become close together and start interacting.

The implementation of such a solution requires an algorithm for designating the correct velocity field to the material points. To achieve that, each material points have additionally defined a domain of interaction. The proposed scheme uses this domain of interaction around each material point for designating the velocity field to that particle.

The algorithm initially checks whether the material points are in the disconnected state based on the specified critical density, below which the material becomes disconnected. This critical value of density and particle mass allow to calculate critical volume for a particle, which is the highest volume a particle can have in a solid state while still being connected to, and thus interacting with the other particles. The domain of interaction is defined as the particle domain scaled to that critical volume. The domain of interaction is a line in 1D MPM variants, a constant square in 2D MPM and uGIMP, a shape changing constant volume rectangle in 2D cpGIMP and a shape changing constant volume parallelograms in 2D CPDI.

Figure 2 shows a schematic of particle domains and domains of interaction for 1D particles. In this figure, particle 1 has a domain, marked with thick dash lines, smaller than its domain of interaction, marked with continues thin lines. Particle 2 is a particle that has reached its domain of interaction and can no longer interact with other particles. Particle 3 and 4 are two contiguous and non-overlapping particles with their domains of interaction crossing over each other. The domain of interaction of contiguous particle can cross over domains of interaction of adjacent particles as long as volume of particle remains below critical volume. On the other hand, the domain of interaction of a particle stops crossing the domain of interaction of the other materials points immediately after that particle reaches its critical volume. Also, at that time the particle domain is exactly the size of domain of interaction. Such a specification of domains of interaction provides a tool for identification of particles that interact together and have common velocity field.

The algorithm designates a velocity field to each particle in the beginning of an MPM step. That allows using the cpGIMP and CPDI for modelling of disconnected granular flow, as being in different velocity fields means that the material points stop interacting. The algorithm designates the velocity fields based on particle domains of interaction. First, it designates particle 1 to velocity filed 1. Then, checks if domain of interaction of particle 1 intersects with any particle. That interacting particle will also have their velocity field set to 1. If any material points remain not assigned to a velocity field, the process for them is repeated, but with velocity field 2, 3 and so on. At the end of the algorithm, all the material points should have one and only one velocity field. The described process of designation of velocity fields is repeated at the beginning of every time step of MPM algorithm.

Figure 3 shows a 1D example of material points disconnection and illustrates how original MPM and cpGIMP simulates disconnected state, with and without velocity field designation to particles. In the left of Figure 3, material points 1 and 2 represents solid material and have intersecting domains of interaction. The solid material represented by those points move towards left. Material point 3 has just separated from the solid part, is disconnected, and its domain of interaction does not have any intersection with domain of interaction of any other material point. This material point moves towards the right. Material points 4 and 5 represent another solid part of the material, have intersecting domains of interaction, and move toward left. The original MPM and cpGIMP simulations use linear elastic material for solid part and approximate the disconnected part to be stress free. Table 1 shows the parameters used in all the simulations.
Table 1 - parameters of MPM and cpGIMP simulations

<table>
<thead>
<tr>
<th>E</th>
<th>(\rho_{\text{initial}})</th>
<th>(\rho_{\text{critical}})</th>
<th>(dt)</th>
<th>Grid spacing</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 kPa</td>
<td>1500 (\text{kg/m}^3)</td>
<td>1400 (\text{kg/m}^3)</td>
<td>0.00002</td>
<td>1 cm</td>
</tr>
</tbody>
</table>

Figure 4 shows the velocity of material point 3 using standard MPM and cpGIMP calculations, with and without velocity field algorithms. The velocity of point 3 changes slightly in the beginning of simulation with original MPM while it remains completely unchanged in the algorithm enriched with the separate velocity fields. The velocity change in the original MPM is caused by interaction between particles in the neighbouring cells and finishes as soon as material points 3 and 2 (see Figure 3), move to the non-neighbouring cells. Furthermore, the original MPM simulation leads to changes in the velocity of material point 3 considerably sooner than the simulation with algorithm using different velocity fields. This is caused by the interaction between material points in the neighbouring cells, which is not prevented by a stress free constitutive model of particle 3. These disconnected-solid interactions depend on the relative positon of particles on the grid and lead to a grid dependent solution. On the other hand, the original MPM simulation enriched with different velocity fields prevents these unwanted interaction of disconnected-solid material points and decrease the grid dependency of original MPM in modelling disconnected state.

Figure 4 also illustrates velocity of material point 3 obtained with cpGIMP calculation. This figure shows that velocity of material point 3, which is disconnected, changes continuously when cpGIMP calculation is performed and proves that disconnected state cannot be modelled with cpGIMP algorithm. On the other hand, cpGIMP simulation with different velocity fields prevents the disconnected material point from interaction and enable cpGIMP modelling.

![Figure 4](image)

Figure 4 - velocity of particle 3 in original MPM and cpGIMP calculation

Figure 5 shows displacement of particle 3 using original MPM and cpGIMP calculations. This figures shows that original MPM and cpGIMP predictions for particle 3 displacement are quite different. On the other hand, the predictions become very similar when the algorithm uses the domain of interactions and different velocity fields.
Original MPM can model gaseous material points without using different velocity fields and the domain of interactions. Figure 6 shows a 1D example of gaseous material points and allows to examine grid dependency of original MPM when modelling gaseous material. In this figure, the distance between the two material points is 2 cm, material point 1 moves toward the right while the other material point is not moving. The domains of interaction of these material points do not intersect, which means these particles are in gaseous state and should not initially interact.

Original MPM simulations predict movements of the material points in Figure 6. These simulations use 2 cm, 1 cm, 0.8 cm and 0.5 cm grid spacing with and without using different velocity fields and the domain of interactions. Figure 7 presents results of these simulations and illustrates displacements of particle 1 (of figure 6). Figure 7 shows that original MPM without using different velocity field and the domain of interactions is greatly grid dependent. This grid dependency reduces considerably with using different velocity field and the domain of interactions when grid density is low or moderate (2cm, 1 cm and 0.8 cm grid). On the other hand, using different velocity field and the domain of interactions have no effect on Original MPM when grid density is high (0.5 cm grid). Original MPM with high grid density prevents material points to interact with each other unless they are very close. This leads to ineffectiveness of domain of interactions and different velocity fields.
Another solutions that can help for dealing with disconnection problem but does not solve it thoroughly is excluding disconnected material points from MPM algorithm and using a separate procedure for moving them. Such an algorithm would help with disconnection problem in all the formulations of MPM but is computationally expansive since crossing of disconnected material points from each other and solid material points should be controlled in each step. Furthermore, this solution may not be able to capture a situation when a disconnection happens within two part of solid material, as illustrated by Figure 8. In Figure 8, material points 1 and 2 are close to each other and have density above critical value. Material points 3, 4 and 5 are also close and above critical density. The gap between these two solid parts indicates that material points 2 and 3 should not interact with each other but different MPM variants will keep them interacting at least for part of calculations without using the separate procedure for disconnected material points.

Conclusion

This paper investigates granular flow in its different stages and proposes modifications allowing for a continuum modelling of these phenomena with Material Point Method. The granular flow behaviour changes significantly between the initiation stage and the disconnected flow state. The paper discusses these variations, and suggests an algorithm allowing for replicating them in different versions of MPM. This algorithm defines a domain of interaction around each material point, finds the points which interact with each other and designates a specific velocity field for these particles. This scheme allows using cpGIMP and CPDI in modelling of granular flow through its disconnected stage, as well as lead to mesh independent simulations.

References


