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Abstract

Granular materials, large collections of macroscopic particles, are something that is commonly found in both nature and industry. Examples of such can be sand, ore, grains, seeds or snow. Simulations of granular materials are important in many industrial cases. It gives an opportunity to study the behavior of the particles as they interact with machinery and gives an indication of how efficient new designs perform.

In some areas, such as vehicle-terrain interaction, plastic deformation of the particles can be an important factor. The Umeå based company Algoryx Simulation can simulate granular materials in their physics engine AGX Dynamics using a nonsmooth discrete element approach (NDEM), but currently lack support for plastic deformation. The purpose of this thesis is to implement a plastic contact model in the source code of AGX Dynamics, such that plastic deformation can be observed.

The implementation was first tested for single particle-particle compression where measured contact forces were compared to theoretical models. Uniaxial compression tests were performed for bulk testing, filling a cylinder with particles and compressing them while monitoring the axial stress and strain.

The results from the single particle compression correspond well to theory, giving the correct plastic deformation for a given contact force and correctly illustrates the effects of changing different model parameters. Plastic deformation could also be observed in the results from bulk testing. Additionally, it was observed that the current version of the implementation is best suited for simulating either very cohesive materials, where particles stick to each other when colliding, or cohesionless materials, where colliding particles are separated after impact. Additional research is needed to study how the separation velocity for colliding particles should be updated in a way that is consistent with the plastic model parameters and experimental results.
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A PGS algorithm for solving the MCP

B Plastic contact algorithm
## Nomenclature

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<td>Identity matrix</td>
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<tr>
<td>c</td>
<td>Damping coefficient</td>
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<td>d*</td>
<td>Effective diameter</td>
</tr>
<tr>
<td>d</td>
<td>Particle diameter</td>
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<tr>
<td>e</td>
<td>Coefficient of restitution</td>
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<tr>
<td>e_H</td>
<td>Non-linearity coefficient</td>
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<tr>
<td>E</td>
<td>Young’s modulus</td>
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<td>E_c</td>
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<tr>
<td>E_p</td>
<td>Plastic Young’s modulus</td>
</tr>
<tr>
<td>f</td>
<td>Force and torque vector</td>
</tr>
<tr>
<td>F_adh</td>
<td>Adhesion, adhesive force</td>
</tr>
<tr>
<td>F_N</td>
<td>Normal contact force vector</td>
</tr>
<tr>
<td>F_hys</td>
<td>Normal hysteric spring force vector</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>g(x)</td>
<td>Gap function</td>
</tr>
<tr>
<td>G</td>
<td>Jacobian of the gap function</td>
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<tr>
<td>ĝ</td>
<td>Rescaled gap function</td>
</tr>
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<td>Ĝ</td>
<td>Rescaled jacobian</td>
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<tr>
<td>k₁</td>
<td>Elastic spring stiffness</td>
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<tr>
<td>k₂</td>
<td>Plastic spring stiffness</td>
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<tr>
<td>k_c</td>
<td>Cohesive spring stiffness</td>
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<tr>
<td>k_N</td>
<td>Normal spring stiffness</td>
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<tr>
<td>M</td>
<td>Mass matrix</td>
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<tr>
<td>m*</td>
<td>Effective mass</td>
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<tr>
<td>n</td>
<td>Non-linearity exponent</td>
</tr>
<tr>
<td>n_d</td>
<td>Dimension of the problem</td>
</tr>
<tr>
<td>N_p</td>
<td>Number of particles</td>
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<tr>
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<tr>
<td>P_b</td>
<td>Bulk plasticity</td>
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<td>Particle plasticity</td>
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<tr>
<td>r</td>
<td>Particle radius</td>
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<tr>
<td>s</td>
<td>Symbol to denote a sign</td>
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<tr>
<td>v</td>
<td>Linear and angular velocity vector</td>
</tr>
<tr>
<td>v_f</td>
<td>Velocity after impact</td>
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<tr>
<td>v_i</td>
<td>Impact velocity</td>
</tr>
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<td>v_IVT</td>
<td>Impact velocity threshold</td>
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<tr>
<td>v_n</td>
<td>Characteristic normal contact velocity</td>
</tr>
<tr>
<td>W_k</td>
<td>Kinetic energy</td>
</tr>
</tbody>
</table>
$W_p$ Potential energy
$x$ Position and orientation vector
$\gamma_r$ Rolling force dissipation parameter
$\gamma_t$ Friction force dissipation parameter
$\delta$ Overlap/contact depth between two bodies
$\dot{\delta}$ Penetration velocity
$\delta_0$ Plastic overlap
$\delta_{adh}$ Adhesive overlap
$\delta_{eff}$ Effective contact depth
$\delta_{max}$ Maximum overlap
$\delta^*$ Maximum overlap limit
$\delta_{min}$ Overlap at maximum cohesive force
$\Delta t$ Time step
$\epsilon_{iter}$ Iteration error tolerance
$\epsilon_{\Delta t}$ Time step error tolerance
$\varepsilon$ Axial strain
$\varepsilon_{max}$ Maximum bulk deformation
$\varepsilon_n$ Normal compliance
$\varepsilon_p$ Bulk plastic deformation
$\eta$ Viscosity constant
$\lambda$ Lagrangian multipliers
$\mu_f$ Friction coefficient
$\mu_r$ Rolling resistance coefficient
$\nu$ Poisson ratio
$\rho$ Density
$\sigma$ Axial stress
$\sigma_1$ Consolidation pressure
$\Sigma$ Compliance regularization matrix
$\tau_n$ Normal force dissipation parameter
$\Upsilon_n$ Damping regularization matrix

**Abbreviations**

- **DEM**: Discrete element method
- **NDEM**: Nonsmooth discrete element method
- **SDEM**: Smooth discrete element method
- **MCP**: Mixed complementary problem
- **PGS**: Projected Gauss-Seidel
1 Introduction

1.1 Background

A granular material is a collection of discrete macroscopic particles that interact locally by interfacial contact forces that are highly dissipative [1]. Examples of such materials could be grains, minerals, pellets or pharmaceutical pills. It has been estimated that more than 50% of the sales in the world deal with products that involve handling of granular materials at some stage [2,3], which makes it very important to be able to predict its behavior. Numerical simulations can be used to optimize a design or machinery that handles granular materials before construction and deployment in order to mitigate errors, improve production performance and reduce maintenance costs. This is important in large scale industries, such as in mining, where manufacturing of machinery often can be time consuming and expensive.

1.2 Discrete element method

One popular method for particle based simulation of granular materials is the discrete element method (DEM) [4]. In DEM, the particles are handled as a system of rigid bodies that interact with each other by modeling of the contact forces. It accurately captures many of the important phenomena of granular media, such as jamming, dilatancy, strong force chains, strain localization and avalanches. When it comes to simulations of granular material in dynamic interaction with different kind of machines (e.g. robots, vehicles, granular transports), DEM can connect the particle based model with a multibody system where the interaction between bodies also can occur via kinematic joints and actuators [5]. The most common approach of discrete element modeling is smooth DEM (SDEM). In SDEM, the velocities are assumed to be continuous in time and the equations of motion can be described by ordinary differential equations. A less used approach is nonsmooth DEM (NDEM), where the velocities are allowed to be discontinuous, and impacts propagate instantly through the system as impulses. This allows for much larger time steps as there is no need to resolve the short impact times [6-8], which could mean that the computational time can be significantly shorter. However, each time step for NDEM is more computationally intense due to a more complicated system of equations. Since the computational time is largely dependent on the system in question, it is not always trivial to predict which of the methods gives the shortest computational time. In general, SDEM is more computationally efficient for systems with soft materials and rapid particle flows while NDEM is more efficient for stiff materials and static or slow flows [7].

1.3 Purpose and goal

Algoryx Simulation, a company located in Umeå, Sweden, successfully combines NDEM and multibody dynamics in their physics engine AGX Dynamics (AGX for short). The current contact model that is used in AGX takes into consideration
model parameters such as elasticity, viscosity, friction and cohesion of the particles. However, the implementation lacks support for plastic deformation of the particles, which limits the possibilities to simulate granular materials where this is an important factor. Examples of such cases are vehicles driving on deformable terrain, excavation, bulldozing and manufacturing of pills by compression of powders. Several regional and global companies have interest in vehicle-terrain simulations since it gives opportunity to make tests of product designs to improve efficiency [6].

The aim of this master thesis is to implement and test a non-linear viscoelastic plastic cohesive contact model that is consistent with NDEM and multibody systems. This includes giving the new contact model a mathematical and algorithmic description based on existing literature for DEM and multibody dynamics, develop a prototype implementation, and construct and perform test for validation and calibration. The prototype implementation has been created in a branch of the source code for AGX (C++) by modifying the existing contact model and introducing new model parameters to include plastic deformation.

1.4 Delimitations

The largest delimitation for the implementation of the plastic contact model is that the geometry of the particles will not explicitly deform when they interact with each other. To explain this, consider Fig. 1 where two spherical particles have collided, undergone plastic deformation and are cohering to each other. To an outside viewer it looks like the particles are no longer completely spherical and that they have a flat circular contact area, see Fig. 1a. However, as seen in Fig. 1b the ”deformation” is instead modeled by a plastic overlap. Since the geometry of the particles remains spherical and does not change, this implies that if they are pulled apart by some external force, the particles will separate and the ”deformation” will be forgotten. This might however not be a huge limitation since many of the applications where the model can be applied have quasistatic material movements, such as terrain deformation and pill compression. In other words, after deformation has occurred, separations of particles are unlikely. For simplicity, only spherical particles of uniform size are used for the simulations. Thus, the intersecting surface between colliding particles is circular. The model can however easily be modified to allow for particles with a more general geometric shape [5].
Figure 1: (a) shows how the particles appear to have deformed and have a circular contact area. However, in (b) we see that their geometry remains spherical and that the particle deformation will be modeled by a plastic overlap.
2 Theory

2.1 Contacting rigid bodies

Before going into the theory behind the contact models, it is important to understand a few key properties about AGX and how it handles particle contacts.

Physical objects in AGX are modeled as rigid bodies, which cannot be deformed and thus retain their shape under the influence of external forces. A rigid body is created by first defining its shape, or geometry. This is done either by using a preset geometry such as sphere, box, or cylinder, or by creating your own using a mesh.

A contact between two rigid bodies is detected when their geometries overlap or coincide. If contact occurs, AGX calculates forces normal to the contact points, which works to separate the bodies. Two geometries can have different number of contact points when colliding. Colliding spheres will always have one contact point, while two colliding boxes can have up to eight. Contact reduction methods can be used to decrease the number of contact points for large systems or complicated geometries. Investigation of contact reduction is however outside the scope of this thesis and has therefore not been considered. Fig. 2 shows a contact between two spherical bodies $a$ and $b$. The contact force at the contact point is split into two tangential, $F_{t1}$ and $F_{t2}$, and one normal component $F_N$. The implementation of the plastic contact model affects only how the normal component of the contact force is calculated, and how it is dependent on the particle overlap $\delta$.

![Figure 2: A contact between two spherical bodies $a$ and $b$, overlapping by a distance $\delta$. $F_N$ is the normal component of the contact force and $F_t$ is the tangential component, which can be split into two parts $F_{t1}$ and $F_{t2}$.](image)

To take into account that geometries can have different materials, a contact material is introduced, where the interaction parameters between two materials is defined. These interaction parameters can for example include Young’s modulus, rolling resistance and friction coefficient.
A granular body system is a set of rigid bodies (particles) with six degrees of freedom. As for regular geometries, the particles can be defined by a material, which is common for all particles within the granular body system. A granular body system handles contacts differently depending on if it collides with another particle or a geometry not belonging to the granular body system [8]. Throughout the rest of the report, "geometries" refers to all other geometries than those defined by the granular body system.

2.2 Viscoelastic contact model

AGX Dynamics uses the non-linear viscoelastic Hertz-Mindlin contact model, which is derived directly from theory of linear elasticity, to handle particle contacts [4]. In this model the normal contact force is split into an elastic spring force and a viscous damping force. The normal contact force is given by

\[ F_N = k_N \delta^{2e_H-1} n + k_N c \delta^{2(e_H-1)} \dot{\delta} n, \tag{1} \]

where \( \delta \) is the contact depth/overlap between contacting bodies, \( \dot{\delta} \) is the penetration velocity, \( e_H \) is a nonlinearity coefficient and \( n \) is the normal unit vector. The nonlinear model uses \( e_H = 5/4 \), while \( e_H = 1 \) reduces Eq. (1) to a linear spring model. For spherical particles, the spring stiffness and damping coefficients are

\[ k_N = \frac{E \sqrt{2} d^*}{3(1-\nu^2)}, \tag{2} \]
\[ c = \frac{4(1-\nu^2)(1-2\nu)\eta}{15E\nu^2}, \tag{3} \]

where \( E \) is the Young’s modulus, \( \nu \) is the Poisson ratio, \( \eta \) is the viscosity constant and \( d^* \) is the effective diameter of the colliding bodies [9]. For particle-particle contacts, the effective diameter is given by \( d^* = (d_1^{-1} + d_2^{-1})^{-1} \) for particles with diameter \( d_1 \) and \( d_2 \). For particle-geometry contacts on the other hand, the effective diameter is simply given by \( d^* = d \).

The normal force between two contacting particles is shown in Fig. 3. Due to the velocity dependent viscous damping, the normal force is larger when loading (pushing the particles together) than when unloading (pulling them apart), leading to energy dissipation. The total dissipated energy is equal to the area of the elliptic shape between the loading and unloading curves. In reality this energy is dissipated as heat, which changes the temperature of the particles and which also can affect material properties [4]. This temperature difference is however neglected in the simulations. When the damping part of the normal force is neglected, for example due to very slow penetration velocities, the normal force will simply be given by the non-linear spring force, as shown in Fig. 4.
To allow for adhesive forces between particles, the contact material parameters adhesion and adhesive overlap need to be introduced. The adhesive overlap, $\delta_{adh}$, determines at which contact depth the normal force is zero while the adhesion, $F_{adh}$, defines the maximum adhesive force for the contact. This is illustrated in Fig. 5, where the viscous damping has been neglected for simplicity.

### 2.3 Viscoelastic plastic cohesive contact model

The plastic model used in this thesis is called the non-linear viscoelastic plastic cohesive Hertz-Mindlin model [10–12]. Similarly to the non-plastic model, the normal contact force is given by

$$F_N = F_{hys} + k_1C\delta^{n-1} \dot{\delta}n,$$  \hspace{1cm} (4)
where \( n = 2e_H - 1 \). Here a hysteric spring force \( F_{hys} \) is used, defined as

\[
F_{hys} = \begin{cases} 
(F_0 + k_1 \delta^n)n & \text{if } k_2(\delta^n - \delta^n_0) \geq k_1\delta^n \\
(F_0 + k_2(\delta^n - \delta^n_0))n & \text{if } k_1\delta^n > k_2(\delta^n - \delta^n_0) > -k_c\delta^n \\
(F_0 + -k_c\delta^n)n & \text{if } -k_c\delta^n \geq k_2(\delta^n - \delta^n_0).
\end{cases}
\]  

(5)

The hysteric spring force is illustrated in Fig. 6a. As for the viscoelastic model, \( e_H = 1 \) gives a linear model, as shown in Fig. 6b.

As the particles start to overlap (\( \delta = 0 \)) they are attracted to each other by a small force \( F_0 \). This force can for example be due to van der Waals forces between very small particles while it for larger particles can be neglected. Thus, \( F_0 = 0 \) is used for this thesis. During initial loading the overlap causes the hysteric force to increase along the slope with stiffness coefficient \( k_1 \), calculated using Eq. (2). From here on, the slope with stiffness \( k_1 \) will be referred to as the \( k_1 \)-branch, while the slopes with stiffness \( k_2 \) and \( k_c \) in Fig. 6 are referred to as the \( k_2 \) and \( k_c \)-branch. At some point, the overlap reaches a maximum value \( \delta_{max} \), which is remembered throughout the whole contact. When the particles start to unload, the force decreases along the slope with stiffness coefficient \( k_2 > k_1 \) and becomes zero at \( \delta = \delta_0 \), which is the plastic overlap of the contact. This means that if no external forces act on the particles at this point, they will remain at rest with overlap \( \delta_0 \). The value of \( \delta_0 \) can be found by using that the \( k_1 \)-branch and \( k_2 \)-branch are equal at \( \delta_{max} \), \( k_1\delta^n_{max} = k_2(\delta^n_{max} - \delta^n_0) \), which gives

\[
\delta_0 = \left(1 - \frac{k_1}{k_2}\right)^\frac{1}{n} \delta_{max}.
\]  

(6)

Reloading from \( \delta_0 \) initially causes the force to increase along the \( k_2 \)-branch but switches to the \( k_1 \)-branch if the overlap exceeds the previous maximum overlap, which is then updated as \( \delta_{max} = \delta \). Unloading below \( \delta_0 \) leads to a cohesive force which reaches its maximum at \( \delta_{min} \). These cohesive forces is used to model how well a granular material sticks together, for example due to wetness and liquid bridges. By unloading even further, the force follows the slope with coefficient \( k_c \). Similarly to \( \delta_0 \), one can calculate \( \delta_{min} \) by using that the \( k_2 \)-branch and \( k_c \)-branch are equal at \( \delta_{min} \), \( k_2(\delta^n_{min} - \delta^n_0) = -k_c\delta^n_{min} \), which gives

\[
\delta_{min} = \left(1 + \frac{k_c}{k_2}\right)^{-\frac{1}{n}} \delta_0.
\]  

(7)

As the particles unload along the \( k_c \)-branch, the maximum overlap is updated as \( \delta_{max} = \delta_{max} - (\delta_{min} - \delta) \) and, if reloaded, the force will increase towards this value with slope \( k_2 \). Observe that \( \delta_{max}, \delta_0 \) and \( \delta_{min} \) are not fixed parameters but variables that depend on the history of the contact.
2.3.1 Effects of changing the stiffness coefficients

As seen in Eq. (2), $k_1$ is linearly dependent on Young’s modulus, which is a measure of the stiffness of a material. Materials with a small Young’s modulus are elastic while materials with a large Young’s modulus are stiff. Granular materials and soils typically have a Young’s modulus in the range 0.4-300 MPa [13–15]. Increasing Young’s modulus (and thus also $k_1$) makes the contact more stiff and makes the particles overlap less for a given contact force.

We define the particle contact plasticity $P_p$ as the ratio between the plastic and maximum overlap, which becomes

$$P_p = \frac{\delta_0}{\delta_{max}} = \frac{1 - \frac{k_1}{k_2}}{2}.$$  \hspace{1cm} (8)

By choosing $k_2 = k_1$ the plastic deformation, $\delta_0$, will become zero which means that the model will become viscoelastic. In this case, $k_c$ will become superfluous since the $k_c$-branch cannot be reached. On the other hand, if the contact plasticity $P_p \rightarrow 1$ then $\delta_0 \rightarrow \delta_{max}$, which is the maximum possible deformation. How the contact plasticity increases in relation to the ratio $k_2/k_1$ can be seen in Fig. 7. We note that using $k_2 > 10k_1$ does not give a significant increase in plastic deformation. This effect can also be seen in Fig. 8 where the hysteric force is plotted for different $k_2/k_1$ ratios.
Figure 7: The particle plasticity as a function of the ratio $k_2/k_1$.

Increasing the value of $k_c$ increases the cohesive force (maximum negative hysteric force) between interacting bodies. A low value means that small external forces are needed to separate two cohering particles while a large value means that large forces are needed. Fig. 9 shows how the cohesion increases for different values of $k_c$. 
relative to $k_1$. Increasing $k_c$ at the same time as $k_2$ gives an even greater cohesive force.

Figure 9: Effects on the hysteric spring force when increasing the value of $k_c$ while keeping $k_1$ constant. Increasing $k_c$ increases the cohesive force of the contact. Here $k_2 = 2k_1$.

2.3.2 Using a variable plastic stiffness coefficient

A more realistic contact behavior would be to let $k_2$ depend on the maximum overlap $\delta_{\text{max}}$, in a way such that the contact becomes stiffer and more plastically deformed for larger previous deformations. This has been implemented by Luding and coworkers \[11, 12\] when using the linear model ($n = 1$). They introduce another model parameter $\delta^*_{\text{max}}$ and let $k_2$ interpolate between $k_1$ and a maximum stiffness $\hat{k}_2$ like

$$
k_2(\delta_{\text{max}}) = \begin{cases} 
k_2 & \text{if } \delta_{\text{max}} \geq \delta^*_{\text{max}} \\
k_1 + (\hat{k}_2 - k_1)\frac{\delta_{\text{max}}}{\delta^*_{\text{max}}} & \text{if } \delta_{\text{max}} < \delta^*_{\text{max}} \end{cases}.
$$

The effects of this is that $k_2$ will increase for increasing overlap, until the maximum overlap limit $\delta^*_{\text{max}}$ is reached. Loading beyond this point will lead to an completely elastic compression where the hysteric force increases along the $k_2$-branch instead of the $k_1$-branch. The effects of loading beyond $\delta^*_{\text{max}}$ for the non-linear model can be seen in Fig. \[10\]. Although a constant value of $k_2$ will be used in this thesis, which is not dependent on the maximum overlap as in Eq. (9), the maximum overlap limit $\delta^*_{\text{max}}$ will still be introduced such that the contact will be completely elastic when loaded beyond this point. This can then later also be used to implement a variable $k_2$ if desired.
If the particles load beyond $\delta^*_\text{max}$, the contact follows the $k_2$-branch which does not lead to any increase in the plastic overlap $\delta_0$.

2.4 Coefficient of restitution

The coefficient of restitution of two colliding bodies is defined as the ratio between their relative velocity after impacting ($v_f$) and before impacting ($v_i$),

$$e = -\frac{v_f}{v_i},$$

known as the Newton impact law [7]. It is commonly assumed that this coefficient is constant for a given material. However, empirical studies show that this is not the case and that it varies with the impact velocity. Fig. 11 shows a theoretical model for the coefficient of restitution (solid curve) and empirical data produced by Bridges et al. [4, 16] (dashed curve), where the restitution was measured for colliding ice spheres at low temperatures. The theoretical expression is calculated using Newton’s equations of motion and is based on the nonlinear viscoelastic model described in section 2.2.
AGX currently uses a user-defined, constant restitution. If an expression for a velocity dependent coefficient of restitution, based on the plastic contact model described in section 2.3, can be determined, this could greatly improve the physics of AGX. Therefore, an attempt to do so will be presented in the following section.

2.4.1 Coefficient of restitution for the plastic contact model

There are no previous studies on how the coefficient of restitution for the non-linear plastic model can be derived, and thus there exist no model to describe this. Singh et al. [12] uses energy conservation to calculate a restitution for the linear plastic model where the viscous damping in Eq. (4) is neglected. By doing so, the restitution becomes an approximation of what would be correct for the model. It might however be a sufficiently good approximation, and to determine if this is the case, a similar approach was used here to calculate the restitution for the non-linear plastic model.

First we assume that the normal force is simply given by the hysteric spring force, i.e. $\dot{\delta} = 0$ in Eq. (4). The hysteric force is shown in Fig. 12 where different points during the contact has been marked. Just before impact, the particles will have a kinetic energy

$$W_{k,A} = \frac{1}{2} m^* v_i^2,$$  \hfill (11)

where $m^*$ is the effective mass and $v_i$ is the impact velocity.

**Figure 11:** Experimental (dashed curve) and theoretical data (solid curve) for the coefficient of restitution as a function of impact velocity (here denoted $g$). [4][16]
The hysteric force during a contact. All kinetic energy before impact (at point A) is completely transferred into potential spring energy as the particles reach their maximum overlap at point B. Energy is then dissipated due to plastic deformation, and the remaining energy is transferred into kinetic energy as the particles unload to the plastic overlap at C. Some of the kinetic energy is transferred to potential spring energy at C, and finally completely to kinetic energy at separation at E.

The kinetic energy is completely transformed into the potential spring energy

\[ W_{p,B} = \int_0^{\delta_{\text{max}}} k_1 x^n dx, \]  

at point B, from which one can solve that

\[ \delta_{\text{max}} = \left( \frac{n+1}{2k_1} m^* v_i^2 \right)^{\frac{1}{n+1}}. \]  

At point C, this potential energy has been transformed into a kinetic energy \( W_{k,C} \) and a dissipated energy due to plastic deformation and is given by

\[ W_{k,C} = W_{p,B} - W_{\text{diss}} = W_{p,B} - \left( \int_0^{\delta_{\text{max}}} k_1 x^n dx - \int_{\delta_0}^{\delta_{\text{max}}} k_2 (x^n - \delta_0^n) dx \right) = \int_{\delta_0}^{\delta_{\text{max}}} k_2 (x^n - \delta_0^n) dx. \]  

This kinetic energy is in turn partially converted to potential energy at point D, such that the kinetic energy at that point is given by

\[ W_{k,D} = W_{k,C} - \int_{\delta_0}^{\delta_{\text{min}}} k_2 (x^n - \delta_0^n) dx. \]
The energy is finally converted exclusively to kinetic energy at separation at point \( E \), where we get

\[
W_{k,E} = \frac{1}{2} m^* v_f^2 = W_{k,D} - \int_{\delta_{\text{min}}}^{0} -k_c x^n dx.
\]  

(16)

The coefficient of restitution then becomes \( e_{\text{plastic}} = \frac{v_f}{v_i} = \sqrt{\frac{W_{k,E}}{W_{k,A}}} \), which after solving the integrals and substituting \( \delta_{\text{max}}, \delta_0 \) and \( \delta_{\text{min}} \) with Eqs. (13), (6) and (7) simplifies to

\[
e_{\text{plastic}} = \sqrt{(n + 1) \left(1 + \frac{(k_2 - k_1)}{k_1} \left(\frac{k_2 - k_1}{k_2 + k_c}\right)^{1/n}\right) - \frac{(k_2 + k_c)}{k_1} \left(\frac{k_2 - k_1}{k_2 + k_c}\right)^{n+1/n} - \frac{k_2}{k_1} n.}
\]  

(17)

Thus, the restitution depends on the plastic model parameters \( k_1, k_2, k_c \) and non-linearity exponent \( n \) as desired. Note that for given model parameters the restitution is constant and does not depend on the impact velocity, which is physically incorrect. Even so, some conclusions can still be drawn from it, see section 4.2.

2.5 Multibody dynamics

The equations of motion of the problem are the Newton–Euler equations of rigid body motion, which form a set of ordinary differential equations and are usually integrated with an explicit time stepper using a small step size. From a computational perspective, the main difference between SDEM and NDEM is related to explicit and implicit integration. In SDEM, the contact forces are modeled as damped springs or more general penalty functions. In NDEM, the Newton–Euler equations are constrained by the Signorini–Coulomb contact law [17], replacing the contact springs. The velocities are no longer assumed time-continuous and are computed globally along with the contact forces by solving the constrained equations of motion for the entire contact network using an implicit time-integration algorithm [7]. In the following sections the system of equations for NDEM will be presented, without going into many details about how it is derived or how to solve it.

2.5.1 Notations

For a rigid body, \( a \), with mass \( m[a] \), the notations \( x[a], e[a], v[a], \omega[a], f[a], \tau[a] \) and \( I[a] \) are used to denote the position, orientation, velocity, angular velocity, force, torque and inertia tensor. These are then bundled and generalized as \( x[a] = \left( x^T[a], e^T[a] \right)^T \), \( v[a] = \left( \dot{v}^T[a], \dot{\omega}^T[a] \right)^T \), \( f[a] = \left( \dot{f}^T[a], \dot{\tau}^T[a] \right)^T \) and \( M[a] = \text{diag}(m[a] 1_{3 \times 3}, I[a]) \). By collecting the components of all bodies in the system, we obtain the global system quantities \( x, v, f \) and \( M \).

The number of bodies and contacts are denoted \( N_p \) and \( N_c \) respectively. Brackets and Roman letters (\( a, b, ... \)) will be used to index a body while parentheses and Greek letters (\( \alpha, \beta, ... \)) are used to index a contact. The gap function \( g(\mathbf{x}) \equiv \)
\((\delta_1, \delta_2, \ldots, \delta_{(N_c)})^T\) measures the overlap between interacting bodies and has a jacobian \(G = \partial g / \partial x\).

### 2.5.2 Numerical integration of nonsmooth discrete element method

The time-discrete equations of motion for all interacting bodies in a NDEM system can be described by the system of equations

\[
Hz + b = w_l - w_u
\]

\[
0 \leq z - l \perp w_l \geq 0
\]

\[
0 \leq u - z \perp w_u \geq 0,
\]

where

\[
H = \begin{bmatrix}
    M & -\hat{G}_n^T & -\hat{G}_l^T & -\hat{G}_r^T \\
    \hat{G}_n & \Sigma_n & 0 & 0 \\
    \hat{G}_l & 0 & \Sigma_l & 0 \\
    \hat{G}_r & 0 & 0 & \Sigma_r
\end{bmatrix},
\]

\[
z = \begin{bmatrix}
v_{i+1} \\
\lambda_{n,i+1} \\
\lambda_{t,i+1} \\
\lambda_{r,i+1}
\end{bmatrix},
\]

\[
b = \begin{bmatrix}
    -Mv_i - \Delta t M^{-1} f_{ext} \\
    \frac{1}{\Delta t} \Upsilon_n \hat{g} - \Upsilon_n \hat{G}_n v_i \\
    0 \\
    0
\end{bmatrix}.
\]

This mixed complementarity problem (MCP) is derived using a time-integration method called the SPOOK stepper \[18\] and can be solved using the iterative projected Gauss-Seidel (PGS) algorithm \[5,7\]. The PGS solving algorithm for the MCP can be found in Appendix A.

Here the subindices \(n, t\) and \(r\) denote the normal, tangential and rolling components while \(i\) denotes the current time step. By solving Eq. (18) we obtain the solution vector \(z\) which contain the new velocities \(v_{i+1}\) and Lagrangian multipliers \(\lambda_{i+1}\). The new positions are updated as \(x_{i+1} = x_i + \Delta t v_{i+1}\). \(w_l\) and \(w_u\) are temporary slack variables, which are variables that are added to an inequality constraint to transform it into an equality. \(u\) and \(l\) are upper and lower limits for \(z\) which follows from the Signorini-Coulomb and rolling resistance law \[7,17\]. In order for the contact model to become non-linear, both the gap function and normal jacobian are scaled as

\[
\hat{g}_{(a)} \equiv s|\delta_{eff,(a)}|^{e_H},
\]

\[
\hat{G}_{(a)}^n = e_H|\delta_{eff,(a)}|^{e_H-1}G_{(a)}^n,
\]

where \(\delta_{eff,(a)}\) is the effective contact depth and \(s = sign(\delta_{eff,(a)})\). See section 3.2 for more details. The diagonal matrices \(\Upsilon_n\) and \(\Sigma = diag(\Sigma_n, \Sigma_l, \Sigma_r)\) contain contact material parameters. They regularize the problem and allow modeling of damping and contact elasticity \[18,19\]. These are given by
\[ \Sigma_n = \frac{4}{\Delta t^2} \frac{\varepsilon_n}{1 + 4 \frac{\varepsilon_n}{\Delta t}} N_c \times N_c, \]
\[ \Sigma_t = \frac{\gamma_t}{\Delta t} 1_{2N_c \times 2N_c}, \]
\[ \Sigma_r = \frac{\gamma_r}{\Delta t} 1_{3N_c \times 3N_c}, \]
\[ \Upsilon_n = \frac{1}{1 + 4 \frac{\varepsilon_n}{\Delta t}} N_c \times N_c. \] 

(22)

where

\[ \varepsilon_n = \frac{e_H}{k_N}, \]
\[ \gamma_n = \frac{e^2_H}{k_N c}, \]
\[ \tau_n = \max(n_s \Delta t, \varepsilon_n/\gamma_n). \] 

(23)

The parameter \( \tau_n \) regulates the dissipation rate of the normal force while \( \gamma_t \) and \( \gamma_r \) regulates the dissipation rate of the forces due to friction and rolling resistance. For \( \tau_n \), a coefficient \( n_s \) in the range 2 – 4.5 is commonly used to ensure numerical stability \[7\].

\( \varepsilon_n \) regulates the normal compliance of the non-overlap constraint. This implies that the contact will be completely stiff if \( \varepsilon_n = 0 \) and more elastic as \( \varepsilon_n \) increases. This becomes evident since if \( k_N \) approaches infinity, so will the normal force according to Eq. (1). For the implemented plastic model, \( k_N \) will alternate between \( k_1, k_2 \) and \( k_c \) depending on the stage in the loading process. See section \[3.2\] for details.

2.5.3 Impact stage

High velocity collisions will be numerically overdamped for the MCP in Eq. (18) \[20\], which means that these collisions need to be solved for using a special impact stage. Contacts with a relative contact velocity that is greater than an impact velocity threshold \( v_{IVT} \) are marked as impacting contacts while those with a relative velocity smaller than \( v_{IVT} \) are marked as resting contacts. The impacting contacts are solved by imposing a velocity constraint using the Newton impact law, which was defined by Eq. (10)

\[ G_n^{(a)} v_+ = -e G_n^{(a)} v_- . \] 

(24)

This will instantly update the velocities and positions of the impacting particles using a user-defined coefficient of restitution without having to calculate contact forces based on contact depth. For resting contacts, the corresponding constraint will be \( G_n^{(a)} v_+ = 0 \) which means than the constraint can be applied to all contacts via the matrix multiplication

\[ G_n v_+ = -E G_n v_-. \] 

(25)
where $E$ is a diagonal matrix with entries $e$ or 0 depending on if the contact is impacting or resting. This means that before the resting contacts are solved for using Eq. (18), we need to solve a similar MCP, substituting the vector $b$ for

$$b_{imp} = \begin{bmatrix} Mv_- \\ -EG_n v_- \\ 0 \\ 0 \end{bmatrix}.$$  (26)

As a rule of thumb, the velocity threshold for impacting particles is given by

$$v_{IVT} = \epsilon v_d / \Delta t,$$  (27)

where $d$ is the particle diameter and $\epsilon_v$ is an error tolerance parameter with a typical value of $0.02 - 0.05$ $[20,21]$.

### 2.5.4 Choice of time step and number of iterations

The timestep for NDEM is set by the characteristic normal contact velocities and gravity acceleration, such that the particles cannot overlap more than a fraction $\epsilon_{\Delta t}$ of their diameter from one timestep to the next:

$$\Delta t \leq \min \left( \epsilon_{\Delta t} d / v_n, \sqrt{2d\epsilon_{\Delta t} g} \right).$$  (28)

For particles with a diameter of 10 mm, $v_n = 0.5$ m/s and $\epsilon_{\text{err},\Delta t} = 0.05$, this yields $\Delta t \leq 10^{-3}$. This is $\sim 1000$ times larger than for SDEM $[20,21]$.

The required number of iterations needed by the PGS-solver to avoid artificial elasticity and slippage has been studied by Servin $[21]$, which led to the empirical rule

$$N_{\text{iter}} = 0.1 N_P^{1/n_d} / \epsilon_{\text{iter}},$$  (29)

where $N_P$ is the number of particles, $n_d = 1, 2, 3$ is the dimension of the problem and $\epsilon_{\text{iter}}$ is an error tolerance.

### 2.6 Uniaxial compression tests

A common method for numerically testing the bulk behavior of granular materials are uniaxial compression tests $[10,22,23]$. These are typically done by filling a cylindrical mould with particles and monitoring the axial stress and strain as the particles are compressed to a certain consolidation pressure. An example of such simulation is shown in Fig. 13. The axial stress is defined as

$$\sigma = F/A,$$  (30)

where $F$ is the force acting on pillar of particles with cross-sectional area $A$. The axial strain $\varepsilon$ is the ratio between the change in pillar height $\Delta h$ to its initial height $h_i$. 

17
\[ \varepsilon = \frac{\Delta h}{h_i} \]  
(31)

Furthermore, the *bulk plasticity* of the granular material can be defined as the ratio of the bulk plastic deformation \( \varepsilon_p \) to the maximum deformation \( \varepsilon_{max} \),

\[ P_b = \frac{\varepsilon_p}{\varepsilon_{max}} = \frac{\Delta h_p}{\Delta h_{max}}. \]  
(32)

Similar to the particle plasticity in Eq. (8), the bulk plasticity \( P_b \) is a measure of how plastic the material is when it comes to bulk behavior.

**Figure 13**: An example of how a simulation of an uniaxial compression test can look like. (a) shows the particle pillar right before compression has started and (b) shows how the particle pillar has been compressed to a certain pressure and the compression plate has been lifted. The particles are color coded by height.
3 Method and implementation

3.1 Contact material parameters of the plastic model

In order to implement the plastic contact model, three new parameters were introduced in the contact material: \textit{YoungsModulusPlastic}, \textit{YoungsModulusCohesive}, and \textit{MaximumOverlapLimit}.

\textit{YoungsModulusPlastic}, \(E_p\), defines the plastic stiffness coefficient as
\[ k_2 = \frac{E_p\sqrt{\delta^*}}{3(1-\nu^2)}. \]
Thus it is defined using the same equation as \(k_1\), but using a different Young’s modulus. Since the stiffness equation is linearly dependent on Young’s modulus, the ratio \(E_p/E\) is equal to the ratio \(k_2/k_1\).

\textit{YoungsModulusCohesive}, \(E_c\), is in the same way used to calculate \(k_c\) using Eq. \(2\). The ratio \(E_c/E = k_c/k_1\) tells us how cohesive the contact will be, as illustrated by Fig. \(9\). Since Young’s modulus is used to describe the stiffness and elasticity of a material, it may be incorrect to name this parameter \textit{YoungsModulusCohesive}, since cohesion has nothing to do with elasticity. However, since \(k_c\) is calculated using Eq. \(2\), and to keep things consistent with the other stiffness coefficients, it has been left this way for now.

\textit{MaximumOverlapLimit}, \(\delta_{max}^*\), is the limit at which the hysteric force stops loading along the \(k_1\)-branch and starts loading elastically along the \(k_2\)-branch as described in section \(2.3.2\).

For the model to be valid it must hold that \(k_2 \geq k_1\), which is equivalent to \(E_p \geq E\). To avoid invalid choices of \(E_p\), the viscoelastic model is used if the user sets a value for \(E_p\) that is smaller than \(E\). The viscoelastic model is also used per default, meaning that if the user does not manually define \(E_p\), \(E_c\) or \(\delta_{max}^*\), there will be no plasticity in the contacts.

There are two existing contact material parameters which are incompatible with the plastic model, namely adhesion and adhesive overlap. To avoid problems with the plastic model the adhesive overlap needs to be \(\delta_{adh} = 0\) m while the adhesion needs to be set to some large value, e.g. \(F_{adh} = 10^9\) N. Setting the adhesion to a large value is simply to avoid limiting the maximum cohesive force of the plastic model in a similar way to what was shown in Fig. \(5\).

The non-linearity coefficient \(e_H\) and Poisson ratio \(\nu\) are currently not a part of the contact material and cannot be changed unless the user has access to the source code. The default values \(e_H = 5/4\) and \(\nu = 0.3\) were used unless stated otherwise.

3.2 Algorithm

The main parts of the algorithm will be mentioned here, while the full algorithm can be found in Appendix B. The algorithm starts by looping over all contacts \(\alpha\) in the system and first checking that \(k_2 \geq k_1\). If this is not the case then \(k_2 = k_1\) is
used, which reverts the model to viscoelastic. If the current contact depth exceeds
the (previous) maximum contact depth and if the maximum overlap limit \( \delta_{\text{max}}^* \) has
not been reached, we then update \( \delta_{\text{max},(a)} = \delta_{(a)} \) and \( \delta_{0,(a)} \) using Eq. (6). This is
followed by three if-statements which calculate the normal compliance \( \varepsilon_n \) and scal-
ing, see Eq. (21) and (23), depending on which branch the particles are loading or
unloading along.

If the particles are loading along the \( k_1 \)-branch, the compliance is updated as
\( \varepsilon_n = e_H/k_1 \), which is what gives elasticity to the contact. The effective contact
depth \( \delta_{\text{eff},(a)} \), defined in Eq. (21), is the depth that is experienced by the solving
algorithm and does not necessarily have to be the same as the actual contact depth
\( \delta_{(a)} \). However, on the \( k_1 \)-branch this is actually the case and thus \( \delta_{\text{eff},(a)} = \delta_{(a)} \).

If the particles are loading or unloading along the \( k_2 \)-branch the compliance is up-
dated as \( \varepsilon_n = e_H/k_2 \). This time the effective contact depth is given by \( \delta_{\text{eff},(a)} = s|\delta_{(a)} - \delta_{0,(a)}|^{1/n} \) where \( s \) is the sign of \( \delta_{(a)} - \delta_{0,(a)} \). The effective contact depth
and a lower compliance than for the \( k_1 \)-branch is what gives the plastic effects and
causes the normal force to be zero when \( \delta_{(a)} = \delta_{0,(a)} \). In other words, at \( \delta_{(a)} = \delta_{0,(a)} \)
the solver will experience no overlap which corresponds to zero normal force. The
absolute value and the sign \( s \) is used to avoid imaginary numbers when \( \delta_{(a)} < \delta_{0,(a)} \)
and the non-linear model, \( n = 3/2 \), is used.

For the \( k_c \)-branch, the compliance is updated as \( \varepsilon_n = e_H/k_2 \) and the effective contact
depth as \( \delta_{\text{eff},(a)} = -\delta_{(a)} \). A negative sign, which also happens for the \( k_2 \)-branch
when \( \delta_{(a)} < \delta_{0,(a)} \), is what tells the solver that the force should be cohesive rather
than repelling.

3.3 Model verification

3.3.1 Single particle compression

As a first stage of testing, simple particle-particle and particle-geometry tests were
performed in order to see if the normal contact force follows the expected behavior.
This was performed by pushing together the bodies and letting them overlap by
manually updating their velocities at each time step and measuring the contact
force between them. The simplicity of the test can be seen in Fig. [14].
Figure 14: The normal contact force is measured when pushing two bodies together and letting them overlap. (a) shows a particle-particle compression and (b) shows a particle-geometry compression.

The main purpose of these tests were to determine if the measured normal contact force follow the mathematical expression for the hysterical force, both for particle-particle and particle-geometry contacts and for several different load- and unload-cases. It was also verified that the model works for four special cases:

1. Contacts using a maximum overlap limit $\delta_{\text{max}}^*$.
2. Reverting to the viscoelastic model when choosing $k_2 = k_1$.
3. That the model works for arbitrary values for the non-linearity coefficient $e_H$. In particular $e_H = 1$ which should give the linear version of the model.

The simulation parameters for the tests can be found in Table [I].
Table 1: The simulation parameters used for the single particle-particle and particle-geometry compression tests.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t$ (s)</td>
<td>Time step</td>
<td>$5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>$N_{\text{iter}}$</td>
<td>Number of PGS iterations</td>
<td>50</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>Density</td>
<td>2000</td>
</tr>
<tr>
<td>$r$ (m)</td>
<td>Particle radius</td>
<td>$5 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$v$ (m/s)</td>
<td>Compression velocity</td>
<td>$5 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$E$ (Pa)</td>
<td>Regular Young’s modulus</td>
<td>$10^6$</td>
</tr>
<tr>
<td>$E_p/E = k_2/k_1$</td>
<td>Ratio between the plastic and regular Y. mod.</td>
<td>1, 2, 10</td>
</tr>
<tr>
<td>$E_c/E = k_c/k_1$</td>
<td>Ratio between the cohesive and regular Y. mod.</td>
<td>0.05, 1</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>Friction coefficient</td>
<td>0.3</td>
</tr>
<tr>
<td>$\tau_n$</td>
<td>Damping</td>
<td>$4.5\Delta t$</td>
</tr>
<tr>
<td>$F_{\text{adh}}$ (N)</td>
<td>Adhesion</td>
<td>$10^9$</td>
</tr>
<tr>
<td>$\delta_{\text{adh}}$ (m)</td>
<td>Adhesive overlap</td>
<td>0</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Rolling resistance coefficient</td>
<td>0.2</td>
</tr>
<tr>
<td>$\delta_{\text{max}}$ (m)</td>
<td>Maximum overlap limit</td>
<td>$1.5 \cdot 10^{-4}, 10^9$</td>
</tr>
</tbody>
</table>

3.3.2 Collision tests and coefficient of restitution

The compression tests were followed by collision tests, where two particles were sent towards each other to collide. The impact velocity threshold described in section 2.5.3 was set to a very large value, $v_{\text{IVT}} = 10^9$ m/s, which restricts the solver to never enter the impact stage. This also implies the user-defined coefficient of restitution ($\varepsilon = 0.5$ per default) is not used when calculating at which velocity the particles should separate after impact. The separation velocity is thus calculated by the solver based on the contact depth and contact forces. The simulated coefficient of restitution was measured for a variety of time steps and impact velocities and compared with Eq. (17). All simulation parameters for the collision tests can be found in Table 2.
Table 2: The simulation parameters used for the particle-particle collision tests.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t$ (s)</td>
<td>Time step</td>
<td>$10^{-9} - 2 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>$N_{iter}$</td>
<td>Number of PGS iterations</td>
<td>50</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>Density</td>
<td>2000</td>
</tr>
<tr>
<td>$r$ (m)</td>
<td>Particle radius</td>
<td>0.0005</td>
</tr>
<tr>
<td>$v_i$ (m/s)</td>
<td>Impact velocity</td>
<td>0.01, 0.1, 1</td>
</tr>
<tr>
<td>$E$ (Pa)</td>
<td>Regular Young’s modulus</td>
<td>$10^6$</td>
</tr>
<tr>
<td>$E_p/E = k_2/k_1$</td>
<td>Ratio between the plastic and regular Y. mod.</td>
<td>2</td>
</tr>
<tr>
<td>$E_c/E = k_c/k_1$</td>
<td>Ratio between the cohesive and regular Y. mod.</td>
<td>1</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>Friction coefficient</td>
<td>0.3</td>
</tr>
<tr>
<td>$\tau_n$</td>
<td>Damping</td>
<td>$4.5 \Delta t$</td>
</tr>
<tr>
<td>$F_{adh}$ (N)</td>
<td>Adhesion</td>
<td>$10^9$</td>
</tr>
<tr>
<td>$\delta_{adh}$ (m)</td>
<td>Adhesive overlap</td>
<td>0</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Rolling resistance coefficient</td>
<td>0.2</td>
</tr>
<tr>
<td>$\delta_{max}$ (m)</td>
<td>Maximum overlap limit</td>
<td>$10^9$</td>
</tr>
</tbody>
</table>

3.3.3 Uniaxial compression

To validate the bulk behavior of the model, simple uniaxial compression tests were performed using a cylindrical mould of 15 mm diameter and 40 mm height, as depicted in Fig. [13]. To fill the cylinder, 5000 particles of 1 mm diameter were randomly generated inside the cylinder in a single time step in order for the particles to quickly reach a static state. After a relaxation time of $t_{relax} = 0.1$ s the total normal contact force $F_{n,tot} = \sum_{\alpha=1}^{N_1} F_{n,\alpha}$ and height of the particle pillar, $h$, had both reached stable values, indicating that the particles had reached a static state. Thereafter, a plate was pressed down on the particles at a constant speed of 20 mm/s while measuring the axial stress and strain, until the particles had been consolidated to a pressure of $\sigma_1 = 5000$ Pa. At this point, the compression plate was moved upwards at the same constant speed, eventually losing contact with the particles.

Two different tests was performed, each consisting of several simulations. The first test focused on testing the repeatability of the model, by running simulations several times using the same model parameters to see if the same results were obtained. Three simulations were done using the same particle packing and three by using different random particle packings. The second test was to study the effects on increasing plastic stiffness $k_2$ to see how the bulk behavior follows the model.

Using Eqs. (28) and (29) with an error tolerance of $\epsilon_{\Delta t} = \epsilon_{iter} = 0.03$, the limits for the time step and PGS-iterations were calculated to $\Delta t \leq 2.5$ ms and $N_{iter} = 57$. To minimize interaction between the particles and the cylinder, the friction and rolling resistance coefficients were set to zero for these contacts. All simulation parameters for the uniaxial compression tests can be found in Table 3.
Table 3: Simulation parameters used for the uniaxial compression tests.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t$ (s)</td>
<td>Time step</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>$N_{iter}$</td>
<td>Number of PGS iterations</td>
<td>75</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>Density</td>
<td>2000</td>
</tr>
<tr>
<td>$r$ (m)</td>
<td>Particle radius</td>
<td>$5 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$v$ (m/s)</td>
<td>Compression velocity</td>
<td>0.02</td>
</tr>
<tr>
<td>$\sigma_1$ (Pa)</td>
<td>Consolidation pressure</td>
<td>5000</td>
</tr>
<tr>
<td>$t_{relax}$ (s)</td>
<td>Relaxation time</td>
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</tr>
<tr>
<td>$E$ (Pa)</td>
<td>Regular Young’s modulus</td>
<td>$10^6$</td>
</tr>
<tr>
<td>$E_p/E = k_2/k_1$</td>
<td>Ratio between the plastic and regular Y. mod.</td>
<td>1–100</td>
</tr>
<tr>
<td>$E_c/E = k_c/k_1$</td>
<td>Ratio between the cohesive and regular Y. mod.</td>
<td>1</td>
</tr>
<tr>
<td>$\mu_f$</td>
<td>Friction coefficient</td>
<td>0.3</td>
</tr>
<tr>
<td>$\tau_n$</td>
<td>Damping</td>
<td>$4.5\Delta t$</td>
</tr>
<tr>
<td>$F_{adh}$ (N)</td>
<td>Adhesion</td>
<td>$10^9$</td>
</tr>
<tr>
<td>$\delta_{adh}$ (m)</td>
<td>Adhesive overlap</td>
<td>0</td>
</tr>
<tr>
<td>$\mu_r$</td>
<td>Rolling resistance coefficient</td>
<td>0.2</td>
</tr>
<tr>
<td>$\delta^*_\text{max}$ (m)</td>
<td>Maximum overlap limit</td>
<td>$10^9$</td>
</tr>
</tbody>
</table>

3.3.4 Terrain deformation test

When the algorithm was completely implemented into the source code, the changes were shared with both Martin Servin at Algoryx, and Viktor Wiberg for use in his master thesis [24]. Servin and Wiberg both performed tests to simulate terrain deformation where a bogie (tracked vehicle) drove over beds of particles such that plastic deformation could be observed. Results presented in this thesis are simulated by Servin, using $\Delta t = 10$ ms, $N_{iter} = 50$, $E = 9 \cdot 10^6$ Pa, $E_p = 9 \cdot 10^7$ Pa, $E_c = 9 \cdot 10^6$ Pa and a particle radius $r = 40$ mm.
4 Results and discussion

4.1 Single particle compression

Fig. 15 shows the normal contact forces measured in the simulation for both particle-particle (a) and particle-geometry compression (b). The red lines are the mathematical expression for the hysteric spring force, defined by Eq. (5). The normal contact force follows the mathematical expression for the hysteric spring force, although slightly larger when loading and slightly lower when unloading. This is expected since during loading, the normal force gets a positive contribution from the viscous damping in Eq. (4). During unloading, the damping force is negative due to a negative penetration velocity $\dot{\delta}$ and thus the contact force becomes smaller than the hysteric force. The maximum force of the particle-geometry is larger by a factor of $\sqrt{2}$ which is due to the difference in effective diameters for particle-particle and particle-geometry contacts. As described in section 2.2 particle-geometry contacts have an effective diameter of $d^* = d$ while particle-particle contacts have $d^* = (d^{-1} + d^{-1})^{-1} = d/2$ (for same-sized particles), giving them a ratio of 2. Due to the square root in Eq. (2), this results in a maximum force which is $\sqrt{2}$ times larger for the particle-geometry contact. Since the implemented code for particle-geometry contacts looks the same as for particle-particle contacts and the contact forces in Fig. 15 looks as expected, only results for particle-particle contacts will be presented in the rest of this section.

![Figure 15](image)

**Figure 15:** The measured contact force (blue dashed curve) along with the mathematical expression for the hysteric spring force (red solid curve), as a function of the overlap. (a) shows the particle-particle contact and (b) the particle-geometry contact.

During bulk simulations, particles will typically load and unload several times without separating which is why such a case also was tested, as seen in Fig. 16. As expected, when the particles are unloaded from point B to point C and then reloaded again, the force increases along the same slope until the previous maximum overlap at point B has is reached. Loading further then causes the force to increase along the slope with stiffness $k_1$. If the particles are unloaded below $\delta_{\text{min}}$ at point E, the
maximum overlap decreases such that the force increases via a different slope (F to G) if reloaded again.

Figs. 17-20 show the four special cases of using a maximum overlap limit, reverting to the viscoelastic model, use of the linear model and cohesionless contacts. There are two different ways of applying cohesionless contacts. In the first, \( E_c \) is set to zero, such that \( k_c \) becomes zero. This, however, causes problems since there currently is no safeguard in the implementation to avoid division by zero when updating the normal compliance as \( \varepsilon_n = c_H/k_c \). Setting \( E_c \) to some small value, for example 1\% of \( k_1 \), will however result in practically cohesionless contacts as seen in Fig. 20a. The other way of applying zero cohesion is by setting \( F_{adh} = 0 \), as seen in Fig. 20b.

The simulations correctly illustrate all the desired effects of changing the various parameters, making the model very versatile. Furthermore the maximum overlap limit can in the future easily be used to implement a variable stiffness coefficient \( k_2 \), as described in section 2.3.2 in addition to simply limiting the plastic deformation as in this work. Whether the variable \( k_2 \) should be a linear interpolation as in Eq. 9 or some non-linear interpolation involving the non-linearity exponent \( n \) is a subject for further studies. Introducing a safeguard in the implementation which allows for \( k_c = 0 \) (and thus zero cohesion) is also something that should be implemented. However, it might actually be favorable to use \( F_{adh} = 0 \) for cohesionless cases, as will be explained in the following section.

**Figure 16:** Measured contact force (blue dashed curve) and mathematical hysteretic spring force (red solid curve), as a function of the overlap. Multiple loadings and unloadings. The particle overlap follows A-B-C-B-D-E-F-G-F-A.

**Figure 17:** Measured contact force (blue dashed curve) and mathematical hysteretic spring force (red solid curve), as a function of the overlap. Using a maximum overlap limit \( \delta^{\text{max}} = 1.5 \cdot 10^{-4} \) m.
Results and discussion

Figure 18: Measured contact force (blue dashed curve) and mathematical hysteric spring force (red solid curve), as a function of the overlap. Confirmation of how the model reverts to the non-plastic viscoelastic model when choosing $k_2 \leq k_1$.

Figure 19: Measured contact force (blue dashed curve) and mathematical hysteric spring force (red solid curve), as a function of the overlap. Confirmation of how the model reverts to the linear version of the model when choosing $e_H = 1$.

Figure 20: Measured contact force (blue dashed curve) and mathematical hysteric spring force (red solid curve), as a function of the overlap. Two methods for removing cohesion from the contacts. (a) shows the effects of using a very small value for $k_c$ and (b) when setting the adhesion to zero.

4.2 Coefficient of restitution

4.2.1 Without using an impact velocity threshold

Fig. 21 shows the simulated value for the coefficient of restitution when the solver is not allowed to enter the impact stage. Using large time steps, the particles stick to each other after colliding and do not separate. That the coefficient of restitution is zero for large time steps is to be expected since the collision cannot be resolved in
time and the contact forces do not accurately act on the particles. For smaller time steps the restitution increases more and more and eventually converges towards the calculated value of Eq. (17), for all impact velocities. Since the calculated value is velocity independent and thus not very physically accurate, it might seem strange that the restitution approaches this value for all impact velocities, since more physically accurate results are expected for a smaller time step. There is however an easy explanation to why this occurs. Since Eq. (17) is calculated under the assumption that the viscous damping part of the normal force can be neglected, one could argue that this would mean that the viscous damping is time step dependent and disappears completely as $\Delta t \to 0$. From Eq. (4) one can see that this clearly should not be the case. However, as explained in section 2.5.2, the diagonal regularization matrix $\Upsilon_n$ is what is used to actually model the damping and this matrix is in fact time step dependent, as a fundamental part of the solving algorithm. As $\Delta t \to 0$, this causes $\Upsilon_n \to 0$, which completely removes damping. From this it can be concluded that Eq. (17) is a correctly calculated expression for the coefficient of restitution under the assumption that viscous damping can be neglected. Although this is a result that currently has no use in the current implementation, it has still been presented and discussed with hope that it will be of use to Algoryx in the future.

4.2.2 Using an impact velocity threshold

Since no usable expression for the restitution could be found, the alternative is to use a user defined constant restitution. This does not come without problems however, as shown in Fig. 22. When applying an impact velocity threshold, the solver should enter the impact stage if $v_i > v_{IVT}$, such that the user defined coefficient of restitution can be applied to update the separation velocities of the particles. However, when a non-zero adhesive force is used and the impact velocity threshold...
(red dashed line) is exceeded, the solver cannot correctly apply the coefficient of restitution, causing the particles to cohere to each other instead of separating. On the other hand, if a zero adhesion is used, this does not happen and the separation velocities are correctly updated. Exactly why the solver cannot correctly apply the restitution for non-zero adhesion is currently unknown, and further studies on this are needed. This means that the current implementation will be best suitable for either simulating cohesive granular materials with a restitution close to zero, or for completely cohesionless granular materials with an arbitrary restitution. For the latter, it would be best to use $F_{adh} = 0$ to apply zero cohesion, in order to avoid problems when applying the restitution during the impact stage.

![Figure 22](image)

**Figure 22:** The coefficient of restitution as a function of particle impact velocity. When using zero adhesion (yellow circles), the solver enters the impact stage and applies the user defined restitution if the impact velocity is larger than the impact velocity threshold (red dashed line). If the adhesion is non-zero (blue asterisk), the solver cannot correctly apply the restitution which results in cohesion between the particles. The used time step is $\Delta t = 1$ ms.

### 4.3 Uniaxial compression

Fig. 23 shows the stress-strain response for the repeatability tests. As can be seen, using both the same and different packings gave very similar results. Variation in the stress-strain curves between the simulations would mean that one would not be able to trust the results and that there is some error in the implementation, but this was not observed.
Joacim Lindberg

Results and discussion

Figure 23: Stress-strain response for repeated simulations using the same particle packing (a) and different random particle packings (b). These simulations were run using $k_2/k_1 = 2$.

Fig. 24 shows the stress-strain response for different values of the plastic stiffness $k_2$. When using $k_2 = k_1$, it can be seen that the axial strain does not return to zero when the compression has been lifted (the particle pillar does not return to its initial height). This is something that one would expect when using $k_2 = k_1$, since the compression would be completely elastic. The reason why this happens is because the porosity of the granular material decreases when compressing, i.e. the particles fill up the empty space between them. This became clear by monitoring the total particle overlap $\delta_{\text{tot}} = \sum_{\alpha} \delta_{(\alpha)}$ and observing that it approached zero after the compression plate was raised, indicating that particles had no plastic overlap. For increasing values of $k_2$, the particle pillar will need to be compressed to a larger axial strain in order to reach the desired consolidation pressure of 5000 Pa. This result was also observed by Morrissey [23] and is expected since an increased ratio $k_2/k_1$ gives an increase in the plastic overlap $\delta_0$, allowing the particles to overlap more at zero normal force. High $k_2/k_1$ ratios causes instability of the particle positions, causing them to shift back and forth inside the cylinder. The instability caused the bulk behavior to lose its plasticity such that the particle pillar nearly returned to its original height after the compression had been lifted, as seen in Fig. 24b. This is not expected and a hypothesis to why it happens will be discussed in the next section. The plastic effects of different ratios are also shown in Fig. 25 and 26, where the pillar height and bulk plasticity is presented.
4.3.1 Instability for large ratios

The reason for why the particles lose their plasticity for large ratios might be due to rapid alternations between the $k_1$ and $k_2$-branch, such that the contacts never settles at a plastic overlap at the $k_2$-branch. To explain what is meant by this, consider Fig. 27, where a theoretical behavior of the hysteric force is presented for a ratio $k_2/k_1 = 100$. If two particles are loaded to point A, the large contact force (along with external forces from other particles) can cause a perturbation in the overlap such that the particles are immediately unloaded to point B, skipping the entire $k_2$-branch. Thus, in a single time step, the particles go from experiencing large repelling forces to large attractive forces. In the following time step, the particles might be reloaded to point C, skipping the $k_2$-branch and yet again experience...
repelling forces. This cycle is then repeated several times, each time decreasing the particle overlap until it becomes close to zero, resulting in an elastic behavior. This would explain why this effect is only seen for large $k_2/k_1$ ratios. Using smaller ratios means that a small perturbation from point A will cause the contact force to decrease to somewhere on the $k_2$-branch. In other words, smaller ratios make it easier to resolve the contact traveling along the $k_2$-branch, such that the contact eventually can settle at a plastic overlap.

![Figure 27: Hypothesis of how the hysteric force behaves for large $k_2/k_1$ ratios. Unloading from A could cause the contact force to immediately decrease to point B, skipping the entire $k_2$-branch. In the next time step, the negative contact force will cause the particles to immediately load to point C, again skipping the $k_2$-branch. Repeating this cycle several times causes the overlap to approach zero, giving an elastic behavior.](image)

This hypothesis is strengthened by Fig. 28 which shows the contact force during a particle collision using a large ratio. Initially, the particles penetrate to a contact depth of $4.5 \cdot 10^{-6}$ m but then quickly starts alternating between the $k_1$ and $k_c$-branch, causing the overlap to decrease towards zero. The negative effects of using a too large ratio could still be observed without much improvement when increasing the number of PGS iterations by a factor 4 or decreasing the time step of a factor 5. Thus, further studies need to be made in order to figure out how to simulate large ratios. In the work done by Morrisey [23], compressions for a ratio of up to $k_2/k_1 = 50$ could be performed without noticing any loss of plasticity. Those simulations were based on SDEM, using a very small time step ($\Delta t = 10^{-6}$ s). It is therefore probable that the loss of plasticity for large ratios would not be observable if the simulations of this thesis had been run with a similar time step. This means that it would be possible to resolve the contacts traveling along the $k_2$-branch and settling at a plastic overlap. Although, it might not even be necessary to use such large ratios since it is clear from both Fig. 7 and 26 that using a ratio of more than 10 won’t lead to a significant increase in plasticity.
Figure 28: The contact force during a particle-particle collision, supporting the hypothesis that loss of plasticity for large $k_2/k_1$ ratios is due to rapid alternation between repelling and attractive forces.

### 4.4 Terrain deformation test

Figs. 29–31 shows the terrain deformation test simulated by Servin, where a bogie weighing more than a metric ton drove over a granular bed. After driving across the bed, the bogie left a lasting track depth of 14 cm. The simulation shows that a ratio of 10 works well for large scale compression. Other than that, the terrain simulation serves more as a means to demonstrate the effects of the model, rather than to obtain qualitative test results.

Figure 29: Overview of the test-scene.
Figure 30: Close up of the bogie driving over the bed.

Figure 31: Overview of the granular bed before (a) and after (b) it was driven over by the bogie. The color scale shows that the bogie left a lasting track depth of approximately 14 cm.
5 Conclusion

A viscoelastic plastic cohesive contact model for particle contacts has been implemented and studied in the physics engine AGX Dynamics. The implementation has proven to be very versatile, allowing the user to easily being able to modify the elasticity, plasticity and cohesion of the contacts, as well as the its non-linearity.

Due to interference with a model parameter from the previous viscoelastic model, the separation velocities of colliding particles are currently not updated correctly, causing unnatural cohesion upon collision. This makes the model best suited for modeling of very cohesive materials or simulations where the movement of the particles are quasistatic. Enclosed compression and terrain deformation are two such cases, which both have been simulated with promising results. Attempting to give the particles too much plasticity can currently result in loss of plasticity due to the contacts not completely resolving in time.

Additional studies need to be made in order to understand how to avoid unnatural cohesion of colliding particles as well as avoiding the previously mentioned loss of plasticity, without having to significantly decrease the time step. Furthermore, the implementation still needs to be compared to real world data by studying how to calibrate the different model parameters.
References


A  PGS algorithm for solving the MCP

Algorithm 1  Projected Gauss-Seidel solver for the mixed complementarity problem
1: if impact stage then
2: \( b_n = -EG_nv \)
3: else if continuous stage then
4: \( b_n = (4/\Delta t)\Upsilon_n g_n - \Upsilon_n G_nv \)
5: pre-step \( v = v + \Delta tM^{-1}r_{ext} \)
6: end if
7: \( q = [-b_n^T, 0, 0]^T \)
8: \( D = diag(GM^{-1}G^T + \Sigma) \)
9: for \( k = 1, \ldots, N_{it} \) and while criteria(r) do
10:   for each contact \( \alpha = 0, 1, \ldots, N_c - 1 \) do
11:     for each contact point \( j \) of contact \( \alpha \) do
12:       \( r_{j,k}^{(\alpha)} = -q_{j,k}^{(\alpha)} + G_{j}^{(\alpha)}v \)
13:       \( \lambda_{j,k}^{(\alpha)} = \lambda_{j,k-1}^{(\alpha)} + D_{j,\alpha}^{-1}r_{j,k}^{(\alpha)} \)
14:       \( \lambda_{j,k}^{(\alpha)} \leftarrow proj_{C_{\mu}}(\lambda_{k}^{(\alpha)}) \)
15:       \( \Delta \lambda_{j,k}^{(\alpha)} = \lambda_{j,k}^{(\alpha)} - \lambda_{j,k-1}^{(\alpha)} \)
16:       \( v = v + M^{-1}G_{j,\alpha}^{T}\Delta \lambda_{j,k}^{(\alpha)} \)
17:     end for
18:   end for
19: end for
B Plastic contact algorithm

Algorithm 2 Implementation of plastic contact model

\begin{algorithm}
\begin{algorithmic}
\State for each contact $\alpha = 0, 1, \ldots, N_c - 1$ do
\State $k_1 = E(2d_\alpha^*)^{0.5}/3(1 - \nu^2)$
\State $k_2 = E_p(2d_\alpha^*)^{0.5}/3(1 - \nu^2)$
\State $k_c = E_c(2d_\alpha^*)^{0.5}/3(1 - \nu^2)$
\State $n = 2e_H - 1$
\State if $k_1 \geq k_2$ then
\State \hspace{1em} $k_2 = k_1$
\State end if
\State if $\delta_{\max,(\alpha)} < \bar{\delta}_{(\alpha)}$ and $\delta_{\max}^* \geq \delta_{(\alpha)}$ then
\State \hspace{1em} $\delta_{\max,(\alpha)} = \bar{\delta}_{(\alpha)}$
\State \hspace{1em} $\delta_{0,(\alpha)} = (1 - k_1/k_2)^{1/n}\delta_{\max,(\alpha)}$
\State end if
\State if $k_2(\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n) \geq k_1\delta_{(\alpha)}^n$ and $\delta_{\max}^* \geq \delta_{(\alpha)}$ then
\State \hspace{1em} $\varepsilon_{n,(\alpha)} = \varepsilon_H/k_1$
\State \hspace{1em} $\delta_{\text{eff},(\alpha)} = \delta_{(\alpha)}$
\State else if $(k_1\delta_{(\alpha)}^n > k_2(\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n))$ and $k_2(\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n) > -k_c\delta_{(\alpha)}^n$ \textbf{or}
\State \hspace{1em} $\delta_{(\alpha)} > \delta_{\max}^*$ then
\State \hspace{1em} $\varepsilon_{n,(\alpha)} = \varepsilon_H/k_2$
\State \hspace{1em} $s = \text{sign}(\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n)$
\State \hspace{1em} $\delta_{\text{eff},(\alpha)} = s|((\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n))^{1/n}$
\State else if $-k_c\delta_{(\alpha)}^n \geq k_2(\delta_{(\alpha)}^n - \delta_{0,(\alpha)}^n)$ then
\State \hspace{1em} $\varepsilon_{n,(\alpha)} = \varepsilon_H/k_c$
\State \hspace{1em} $\delta_{\min,(\alpha)} = (1 + k_c/k_2)^{-1/n}\delta_{b,(\alpha)}$
\State \hspace{1em} $\delta_{\max,(\alpha)} = \delta_{\max,(\alpha)} - (\delta_{\min,(\alpha)} - \delta_{(\alpha)})$
\State \hspace{1em} $\delta_{0,(\alpha)} = (1 - k_1/k_2)^{1/n}\delta_{\max,(\alpha)}$
\State \hspace{1em} $\delta_{\text{eff},(\alpha)} = -\delta_{(\alpha)}$
\State end if
\State $s = \text{sign}(\delta_{\text{eff},(\alpha)})$
\State $\tilde{g}_{(\alpha)} = s|\delta_{\text{eff},(\alpha)}|e_H$
\State $G_{n,(\alpha)} = e_H|\delta_{\text{eff},(\alpha)}|e_{H-1}G_{n,(\alpha)}$
\State end for
\State Run PGS algorithm (Appendix A)
\end{algorithmic}
\end{algorithm}