Contact enforcement methods comparison in DEM context: application for railway ballast shear test

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Abstract. In the Discrete Element Method (DEM) analysis the major difficult consists in the treatment of contacts, as there are multiple approaches and dependencies in relation to the particle form, space search as well as several interface laws. In this work, two distinct contact enforcement methods are compared: the classical penalty-based and the barrier method. The former is available in Rocky DEM commercial software and the latter is implemented in the academic code GIRAFFE. Both methods are compared with respect to their capabilities, advantages and limitations. A classical shear box test is used as a comparison basis. The granular material tested is a sample of railway ballast.

Keywords: DEM; Contact; Railway ballast

1 Introduction

The shear box test is a technique for observing the mechanical behavior of a material when imposing shear stress. This test involves placing the material in a confined box, applying pressure through a lid and then moving the lower part of the box at a constant rate while measuring the lateral force required to prescribe such a movement. In railway research, this test is crucial for predicting the maximum shear stress that the configuration of railway ballast can withstand, thereby optimizing track dimensions. In a 2018 study, Estaire and Santana [1] demonstrated that larger shear boxes are better suited for railway ballast due to its large granular size. Since testing with larger shear boxes requires heavy equipment with good precision, simulations of shear boxes are a way to reduce costs and represent the complex shear behavior in granular media. In order to simulate a shear box test, the user requires consideration of ballast movement, geometry, and the system overall void ratio, emphasizing the Discrete Element Method (DEM) as a powerful tool for such analyses.

Idealized by Cundall and Strack [2] as a mean to predict the movement of rock blocks within fragmented massifs, the Discrete Element Method (DEM) is a well-established approach for modeling granular physics. In first applications, particles were represented as discs or spheres, and simulations relied on classic Newtonian equations using explicit numerical methods. Later, one can find DEM versions that support general polyhedra, as developed by Neto and Wriggers [3], and even non-uniform rational B-Splines (NURBS) surfaces, as conceived by Craveiro et al. [4], solving the system equations by implicit or explicit numerical methods.

DEM modelling is often approached in two ways: the classical penalty method, which measures normal forces based on the depth of overlap between objects, and the barrier method, which restricts penetration between objects, causing normal forces to increase inversely with the smallest distance between them.

Hence, this article compares these two methods using two different software implementations.

Firstly, Rocky DEM™, a commercial software created by ESSS and currently developed by ANSYS. Rocky DEM™ is a popular tool that utilizes explicit integration schemes to obtain the simulation's output. Explicit integration schemes, though performing simplicity to solve, require a small time-step as they are not unconditionally stable (from the numerical point of view).

Secondly, GIRAFFE, an academic software developed by Prof. Dr. Alfredo Gay Neto and co-workers that employs a barrier method coupled with a boundary curve to enforce physical constraints. GIRAFFE utilizes implicit time-integration, which, although computationally expensive, permits larger time-steps by verifying the acceptability of new configurations against previous and subsequent frames.

2 Interface Law Methods

This work focuses on the Hertzian contact law, where the normal repulsion between two contacting particles is proportional to the overlap (for penalty-based methods) or the displacement from the contact activation threshold (for barrier methods), raised to the power of 1.5, for more details on Hertzian contact theory, please refer to Johnson [5]. Additionally, a damping coefficient dependent on the velocity of contact is included. Although the software employ different DEM approaches in their analyses, it is possible to simulate the same contact laws in both.

2.1 Rocky DEM™

In Rocky DEM™, the Hertzian normal force law is expressed by eq. (1):

$$F_n = K_h {s_n}^{\frac{3}{2}} + C_h {s_n}^{\frac{3}{2}} \dot{s}_n, \tag{1}$$

where K_h is the Hertzian stiffness coefficient, obtained through eq. (2), C_h is the Hertzian damping coefficient, obtained through eq. (5), s_n is the normal overlap value and $\dot{s}_n$ is the time derivative of the normal overlap.

$$K_h = \frac{4}{3} E^* \sqrt{R^*}, \tag{2}$$

with E^* and R^* obtained from eq. (3) and eq. (4):

$$\frac{1}{E^*} = \frac{1 - {\nu_1}^2}{E_1} + \frac{1 - {\nu_2}^2}{E_2}, \tag{3}$$

$$\frac{1}{R^*} = \frac{2}{L_1} + \frac{2}{L_2}, \tag{4}$$

where E is the Young's modulus, ν is the Poisson's ratio, and L represents the sieve size of the particles, with indices 1 and 2 referring to the parameters of the two particles in contact. The sieve size, as defined in [6], is the dimension of the smallest square aperture through which the particle can pass.

The damping coefficient C_h is given by:

$$C_h = \eta \sqrt{5 m^* K_h}, \tag{5}$$

where m^* is the effective mass obtained by the harmonic average of the masses of the two particles in contact and η is the damping ratio of the material.

Meanwhile, the tangential force between particles is obtained through a linear spring Coulomb model, described by eq. (6).

$$\vec{F}_\tau^t = min(|| \vec{F^t}_{\tau,e} ||, || \mu \vec{F}_n^t ||) \frac{\vec{F}_{\tau,e}^t}{|| \vec{F}_{\tau,e}^t ||}, \tag{6}$$

where $\vec{F}_n^t$ is the value of the normal force in the current time-step, μ is the friction coefficient and $\vec{F}_{\tau,e}^t$ is obtained from eq. (7).

$$\vec{F}_{\tau,e}^t = \vec{F}_\tau^{t-\Delta t} - K_h r_K \Delta \vec{s}_\tau, \tag{7}$$

in which r_K is the tangential stiffness ratio, defined as the ratio between the tangential stiffness K_t and the normal hertzian stiffness K_h, $\vec{F}_\tau^{t-\Delta t}$ is the value of the tangential force in the previous time-step and $\Delta \vec{s}_\tau$ is the tangential relative displacement of the particles during the timestep.

2.2 GIRAFFE

In Giraffe, the equivalent normal force f_n is obtained through eq. (8).

$$\begin{cases} f_n = 0, & \text{if } g_n \geq \bar{g}_n, \\ f_n = \epsilon_1(\bar{g}_n - g_n)^{n_1}, & \text{if } \bar{\bar{g}}_n \leq g_n < \bar{g}_n, \\ f_n = \epsilon_2 g_n^{n_2} + c_2, & \text{if } g_n < \bar{\bar{g}}_n, \end{cases} \tag{8}$$

here ϵ_1 is analogous to a stiffness coefficient, c_2 and ϵ_2 are a constant that maintains the equations matching conditions, n_1 and n_2 are define the shape of the interface law, $\bar{g}_n$ and $\bar{\bar{g}}_n$ are thresholds respectively dividing the domains of no contact, physical constraint contact, and the barrier method, and g_n is the smallest distance between the two analysed particles.

To reach Hertzian contact, in this article we set n_1 to 1.5. The barrier form n_2 is set to -1.

The normal damping force is given by eq. (9).

$$f_d = 2\eta\sqrt{-\frac{df_n}{dg_n}\frac{m_A m_B}{m_A + m_B}}\dot{g_n}, \tag{9}$$

where η is the damping ratio, the indices A and B refer to the properties of different particles in contact and $\dot{g_n}$ refer to the relative velocity in normal direction.

The trial tangential force ${f_t}^{try}$ is initially calculated using eq. (10) and then evaluated against the Coulomb limit, as done in eq. (11), to determine the tangential force f_t.

$${f_t}^{try} = \epsilon_t g_t + c_t \dot{g}_t, \tag{10}$$

where ϵ_t is the tangential stiffness coefficient, c_t is the tangential damping coefficient, and g_t is the tangential gap.

$$\begin{cases} f_t = {f_t}^{try}, & \text{if } f_t \leq f_n\mu_s, & \text{when no sliding occurs between the contacting pair during evaluation,} \\ f_t = f_n\mu_d, & \text{if } f_t > f_n\mu_s, & \text{when sliding occurs between the contacting pair during evaluation,} \end{cases} \tag{11}$$

where μ_s is the static friction coefficient and μ_d the dynamic friction coefficient. A more detailed explanation can be obtained in the work of Neto and Wriggers [3]

2.3 Interface law compatibility algorithm

To compare simulations between the two aforementioned software, it is necessary to export the input from one software into the other. To achieve this, we devised an export algorithm that can adapt a simulation configuration from Rocky DEM™ in a certain time-step to GIRAFFE input format.

Since Rocky DEM™ relies on penetration to evaluate contact, the size of the exported particles is reduced to 99% of their original value to ensure that no penetration takes place, as this is not acceptable when handling contact with barrier-based methods. This adjustment is sufficient to account for the overlap, given that we are working with stiffness coefficients ϵ_1 on the order of $10^9 N/m^{1.5}$. The contact will then be calculated in GIRAFFE algorithm for contact detection, in this case a coarse search of a Verlet list of the bounding volumes, a sphere with a radius 5% bigger than that of the sphere that circumscribes the particle, if contact between spheres is detected, then a second coarse search will be done with a Verlet list of each particle part (vertices, edges and faces), this time using bounding volumes (spheres, cylinders or plane extrusion respectively for each particle part mentioned) and only then a refined search for each part that contact was identified, so that the location of contact is detected.

Additionally, because Rocky DEM™ evaluates contact using parameters specific to the contacting pair, the algorithm will create one interface per possible contacting pair, defining the first threshold $\bar{g_n}$ as 1% of the sum of the sieve sizes of the pair divided by 10 and the second threshold $\bar{\bar{g_n}}$ as $0.2\bar{g_n}$. This ensures that the particles remain outside the barrier domain in GIRAFFE, preventing the simulation from failing due to excessive contact forces, maintaining the use of the interface law in its physical-related interpretation (at least in the beginning of the simulation).

The normal force coefficient ϵ_1 is calculated in the same manner as K_h in eq. (2). Ensuring that the normal force will have the same module in both given a gap equal to the overlap (before reaching GIRAFFE second threshold $\bar{\bar{g}}$). For the damping, Rocky DEM™ uses the coefficient of restitution ε to define it's damping ratio η, as in ESSS [6]. To achieve minimal restitution, which is the most plausible scenario for a shear box test, the restitution coefficient is set to 0.1, resulting in a value of η equal to 4.807. For GIRAFFE, the damping will be set to nearly critical, with a damping ratio η of 0.9.

Table 1 presents the fixed parameters for the particles and boundaries simulated in GIRAFFE and Rocky DEM™.

Table 1. Coefficients in constitutive relations

Constitutive relation	Nomenclature	Giraffe Value	Rocky DEM™ Value
Static friction coefficient	μ_s	0.7	0.7
Dynamic friction coefficient	μ_d	0.6	0.6
Tangential stiffness ratio	r_K	0.05	0.05
Damping ratio	η	0.9	4.807
Particle Young's Modulus	E	5 GPa	5 GPa
Particle Poisson's ratio	ν	0.2	0.2
Boundary Young's Modulus	E	70 GPa	70 GPa
Boundary Poisson's ratio	ν	0.3	0.3

3 Numerical Examples

In this section, we present examples that illustrate each software's capabilities and characteristics.

3.1 Cube being pressed

To better illustrate the barrier method, in this simulation a cube with sides of 6,0624 cm was dropped inside a box. Then, a lid weighing 1 kg dropped over the cube and remained until the simulation reached equilibrium. Finally, the lid exerted a displacement towards the cube at a fixed velocity of 1 cm/s over 2s, performing now a dynamic test, though with a pace comparable to a semi-static one, in a way that the inertia effects don't become relevant, and the force required to do so was measured and plotted against the distance traveled by the lid. The simulation is done by dropping the particle (cube) from a location different from the equilibrium because, and this is also valid for Rocky DEM, the exact position of a particle is not always known with ease prior to the beginning, as it is a function of the contacts that will take place.

Table 2 show the parameters adopted in this simulation:

Table 2. Parameters for Cube being pressed

Parameter	Value
ϵ_1	1.447E6 $N/m^{1.5}$
$\bar{g}$	0.599
$\bar{\bar{g}}$	0.1198 mm
ρ_{cube}	2620 kg/m^3
Gravitational field intensity	9.81 m/s^2

From the data in Table 2, it's possible to predict the maximum displacement of the lid in the simulation by discovering the gap available for displacement in the equilibrium state, as GIRAFFE does not tolerate penetration and beyond this point, an overlap would occur. As in this simulation there will only be face-face contacts, and GIRAFFE degenerates this kind of contact to pointwise interactions, as demonstrated by Neto and Wriggers [3], there will be four forces, one at each vertex of the cube superior face, of equal value resisting the movement imposed by the lid on the cube. By using eq. (8) to calculate the space between the cube and the lid, as well as the space between the cube and the box, it's possible to determine the gap. The results are detailed in eq. (12) and eq. (13).

$$S_{lid-cube} = \bar{g} - \frac{m_{lid}g}{4\epsilon_1} = 0.597578mm, \tag{12}$$

$$S_{cube-box} = \bar{g} - \frac{m_{lid}g + \rho_{cube}V_{cube}g}{4\epsilon_1} = 0.597069mm. \tag{13}$$

where S stands for the gap between objects and V_{cube} is the cube's volume.

In Fig. 1 we have GIRAFFE solution of the problem. In this output the lid displaced by 1.194647 mm, exactly as expected.

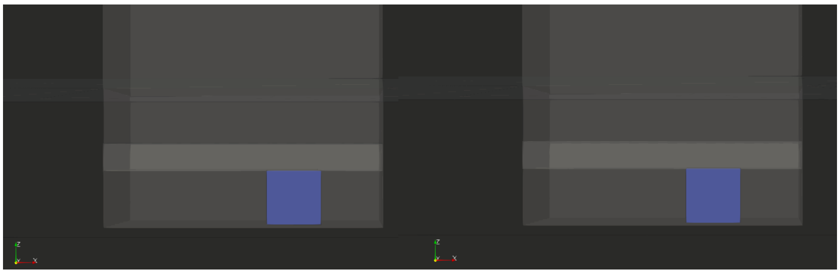

Figure 1. Cube being pressed on GIRAFFE, post processing done in Paraview™, (left) simulation at equilibrium, (right) final output

In Fig. 2 we present the force vs. lid displacement curve, setting zero as the equilibrium coordinates of the lid.

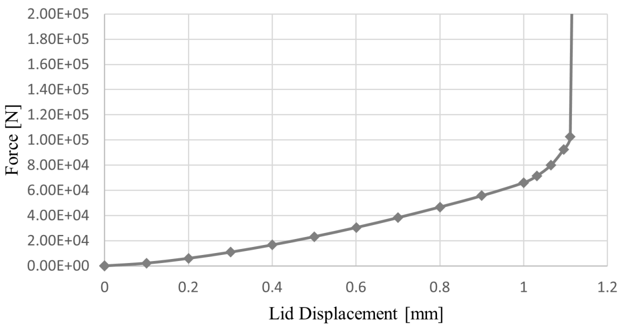

Figure 2. Force vs. lid displacement curve in GIRAFFE

The hybrid-barrier behavior can be observed in Fig. 2. Note that the barrier method keeps elevating the force in order to repel the other body in contact and refrain a penetration from occurring.

3.2 Simplified shear box test

In order to compare both software, a simplified shear box test was developed. Moraes et al. [7] has demonstrated that Rocky DEM™ is capable of performing such a test. Using the interface law compatibility algorithm, we aim to replicate these results in GIRAFFE using a dataset of 90 different ballast samples extracted from the work of Moraes et al. [7] and simplified to a convex shape of 24 faces. Table 3 presents the simulation parameters. Initially, the simulation was conducted in Rocky DEM™. Particles were randomly inserted into the box, and once all particles were positioned, the lid was allowed vertical movement. A gradually increasing vertical force was applied to the lid for 4 seconds, reaching a maximum of -360 N, equivalent to 4 kPa of pressure on the particle bed. Afterward, the lower half of the box began moving at a velocity of 1 cm/s. Once the simulation is concluded, the data was exported to GIRAFFE, using the previously described algorithm, at the time-step just before the lateral movement began, ensuring the particle bed geometry was preserved. After that, the simulation was resumed on GIRAFFE.

The simulations setup can be seen in Fig. 3 for Rocky DEM ™ and in Fig. 4 for GIRAFFE, the output force necessary for the movement can be seen in Fig. 5.

Table 3. Parameters for simplified shear box test

Parameter	Value
Pressure on lid	4 kPa
Lower box velocity	1 cm/s
Number of particles	462
$\rho_{particles}$	2620 kg/m^3
Gravity	9.81 m/s^2
Simulation End	1.65338 s

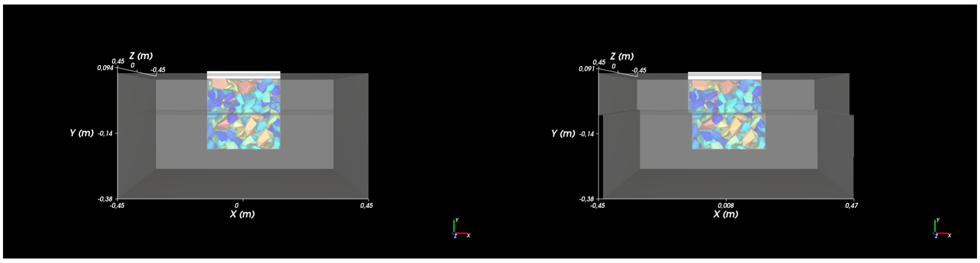

Figure 3. Simplified shear box test on Rocky DEM™, (left) simulation at equilibrium, (right) final output

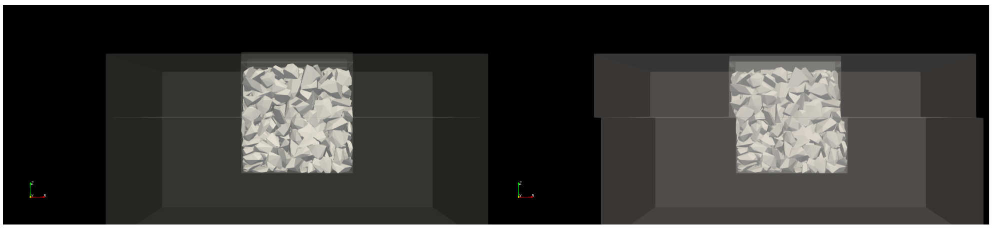

Figure 4. Simplified shear box test on GIRAFFE, post processing done in Paraview™, (left) simulation at equilibrium, (right) final output

To simulate 1.65338 seconds, GIRAFFE required 21 hours and 26 minutes, utilizing 22 out of 24 processors on an Intel(R) Xeon(R) W-2265 CPU @ 3.50 GHz. In contrast, Rocky DEM™ completed the simulation in 9 minutes and 32 seconds, using 23 processors on the same computer. While both simulations show similar curves initially, GIRAFFE allowed some ballast to escape the box after the time frame 1.65338 seconds, compromising the reliability of data beyond this time step. Reducing the time discretization in a new simulation might resolve this issue, albeit at the cost of increased computational time.

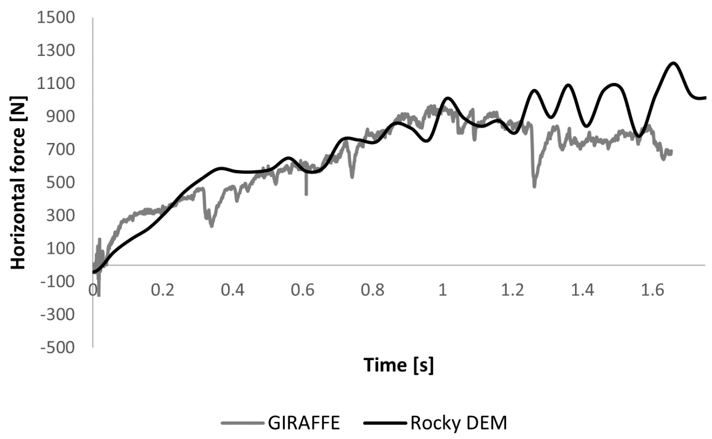

Figure 5. Horizontal force vs Time curve for simplified shear box text in GIRAFFE (Grey) and Rocky DEM^{TM} (Black)

4 Conclusions

We compared DEM simulations employing distinct software and two interface laws, and through an algorithm, simulated the same study on both, obtaining similar results. This assessment confirms the validity of both approaches in DEM modeling. However, it was observed that GIRAFFE's simulations, partly due to its reliance on an implicit integration scheme, cannot efficiently handle a high number of particles within a reasonable solving time. Therefore, constructing large shear box tests using this software is currently impractical, although smaller shear boxes can be simulated. In contrast, Rocky DEM^{TM}, as shown in the work by Moraes et al. [7], efficiently simulated a large shear box involving convex polyhedrons within a reasonable solving time, making the software suitable for such tasks. Future works on GIRAFFE intend to insert aspects related to the computational efficiency, such as explicit method implementation and parallelization of the processing (via GPU).

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