ON THE FRICTION AND CONTACT MODELING METHODS USED IN SIMULATIONS OF GEOMECHANICAL TESTS

by

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ON THE FRICTION AND CONTACT MODELING METHODS USED IN SIMULATIONS OF GEOMECHANICAL TESTS

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This thesis presents a validation of two methods usually used in simulations of granular material. Algorithms based on those methods are implemented in an open-source software, called Chrono. The algorithms were validated against experimental data found in literature or provided by our collaborators. Both approaches can be classified as discrete element methods (DEM), since they describe a mechanical system in a discrete fashion (i.e. positions and orientations of each body, belonging to mechanical system, is tracked separately). However, they can be distinguished based on the way they handle the aspects of friction and contact. First method treats bodies as they were rigid and imposes a non-penetration complementarity condition on colliding bodies. Thus, it is called DEM via complementarity, or DEM-C. Second one allows inter-penetration between colliding bodies and puts a penalty-type condition on contact force acting between them. This method is called DEM-P, from penalty.

In this thesis algorithms based on DEM via penalty and complementarity were validated against often-encountered geomechanical tests, namely against cone penetration, standard triaxial and direct shear tests. It turned out that those two methods can be successfully used in such simulations. This outcome is quite remarkable, since methods handle friction and contact using vastly different ways, either from physical or numerical angles.

Apart from reproducing those geo-mechanical tests numerically, a performance analysis was carried out. It showed that calculations using DEM-P method were much faster in simulating standard triaxial test. The performance of methods was comparable in cone penetration test simulations. DEM-C outran penalty approach when it came to the execution time od direct shear test. Speed-ups seen in standard triaxial and cone penetration tests were
caused by the opportunity of taking longer time steps. This opportunity was possible due to the relaxation of particles stiffness (their Young’s modulus was about 1000 times smaller than in reality).

Moreover, a couple of sensitivity analyses were conducted on. Our aim was to show to what extent simulated mechanical system was sensitive to a change of certain parameters’ value. For example, we checked the response of mechanical system for different values of coefficient of friction in cone penetration and standard triaxial tests. Subject of the analysis in direct shear test simulation was e. g. shearing speed. Report on each of the numerical tests is available on–line, as well as the source codes of all the numerical tests carried out.
ABSTRACT

This thesis presents a validation of two methods usually used in simulations of granular material. Algorithms based on those methods are implemented in an open-source software, called Chrono. The algorithms were validated against experimental data found in literature or provided by our collaborators. Both approaches can be classified as discrete element methods (DEM), since they describe a mechanical system in a discrete fashion (i.e., positions and orientations of each body, belonging to mechanical system, is tracked separately). However, they can be distinguished based on the way they handle the aspects of friction and contact. First method treats bodies as they were rigid and imposes a non-penetration complementarity condition on colliding bodies. Thus, it is called DEM via complementarity, or DEM-C. Second one allows inter-penetration between colliding bodies and puts a penalty-type condition on contact force acting between them. This method is called DEM-P, from penalty.

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1 DESCRIPTION OF METHODS

1.1 Penalty Based Discrete Element Method

In simulations using penalty based Discrete Element Method (DEM-P) [1, 2] colliding bodies share more than one point. Thus, to every contact an inter-penetration gap, called $\delta_n$, can be assigned. This overlap as well as relative velocity between those two colliding bodies are used in calculating the contact force. Formulas used in computing normal and tangential force components ($F_n$ and $F_t$, respectively) were presented in Eq. (1.2).

\begin{align*}
F &= F_n + F_t \\
F_n &= F_n n = (k_n \delta_n - \gamma_n v_{rel,n}) n \\
F_t &= -k_t \delta_t - \gamma_t v_{rel,t}
\end{align*} \quad (1.1, 1.2a, 1.2b)

A unit normal vector, $n$, defines orientation of contact surface, see Fig. 1.1. Normal ($v_{rel,n} = v_{rel,n} n$) and tangential ($v_{rel,t}$) components of relative velocity can be obtained from Eqs. (1.3). Vectors $v_k$, $\omega_k$ and $s_k$ are defined as linear velocity, angular velocity and vector connecting center of mass of $k$-th body with contact point.

\begin{align*}
v_{rel} &= v_j + \omega_j \times s_j - v_i - \omega_i \times s_i \\
v_{rel,n} &= (v_{rel} \cdot n)n = v_{rel,n} n \\
v_{rel,t} &= v_{rel} - v_{rel,n} = |v_{rel} - v_{rel,n}| t = v_{rel,t} t,
\end{align*} \quad (1.3a, 1.3b, 1.3c)

where $t$ is a unit vector.

Different formulas can be used in calculating quantity $\delta_t$, called tangential contact displacement. They depend on the choice of tangential history model. In this work, single- and multi-step models of tangential history were described (see also [3, 4]). In the former
Figure 1.1: Bodies $i$ and $j$ in contact. Plane tangent to two bodies colliding (with normal $\mathbf{n}$), as well as penetration gap /($\delta_n$) were shown in the picture. Quantities needed in calculations of relative tangential velocity were also visualized: $\mathbf{v}$ – linear velocity; $\omega$ – angular velocity; $\mathbf{s}$ – vector connecting center of mass of one colliding body with contact point.

one, $\delta_t = \mathbf{v}_{rel,t} \times \Delta t$, and tangential displacement vector, $\delta_t$, is always parallel to the current relative tangential velocity. Hence, $\mathbf{F}_t$ can be expressed as:

$$\mathbf{F}_t = F_t \mathbf{t} = (-k_t \delta_t - \gamma_t \mathbf{v}_{rel,t}) \mathbf{t}$$  \hspace{1cm} (1.4)$$

When it comes to the multi-step model of tangential history, information from previous time steps is needed to compute $\delta_t$. Namely, information from all recent consecutive time steps in which bodies were in contact has to be taken into account.

$$\delta_t^m = \delta_t^{m-1} + \mathbf{v}_{rel,t} \times \Delta t$$  \hspace{1cm} (1.5a)$$

$$\delta_t = \delta_t^m - (\delta_t^m \cdot \mathbf{n}) \mathbf{n}$$  \hspace{1cm} (1.5b)$$

where $m$ is a number of consecutive time steps during which bodies were in contact; $\mathbf{n}$ is a unit normal vector in current time step and $\delta_t^0 = \mathbf{0}$. Since bodies can touch each other for a couple of successive time steps, their relative position and orientation can change. Thus, vector $\delta_t^m$ does not have to lie on a plane tangential to two colliding bodies in current time.
step. To clamp $\delta_m^m$ on the tangent plane, projection shown in Eq. (1.5b) is needed. Vector $\delta_t$ obtained from Eqs. (1.5) might not be parallel to $v_{rel,t}$.

Parameters $k_n$, $k_t$, $\gamma_n$ and $\gamma_t$ represent stiffness and damping coefficients describing components of the contact force. They depend on elastic parameters of colliding bodies and coefficient of restitution. In Hertzian contact model $k$’s and $\gamma$’s additionally depend on $\delta_n$. Parameters in Hookean model do not depend on $\delta_n$; instead they depend on parameter called characteristic velocity, $V_{ch}$. In every simulation presented in this thesis, velocities of bodies did not exceed 1.0 m/s, thus characteristic velocity was set up to this value and was constant, $V_{ch} = 1$ m/s. Formulas used in calculating stiffness and damping parameters in Hookean and Hertzian models were presented below:

**Hookean contact model**

\[
\begin{align*}
k_n &= T_n \left( \frac{m_{eff} (V_{ch})^2}{T_n} \right)^{0.2} \\
k_t &= k_n \\
\gamma_n &= \sqrt{\frac{4 m_{eff} k_n}{C_n}} \\
\gamma_t &= \gamma_n,
\end{align*}
\]

where

\[
\begin{align*}
T_n &= \frac{15}{16} \sqrt{R_{eff} Y_{eff}} \\
C_n &= 1 + \left( \frac{\pi}{\ln(c_r)} \right)^2
\end{align*}
\]

**Hertzian contact model**

\[
\begin{align*}
k_n &= \frac{2}{3} S_n \\
k_t &= S_t
\end{align*}
\]
\[ \gamma_n = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_n m_{eff}} \tag{1.8c} \]
\[ \gamma_t = -2 \sqrt{\frac{5}{6}} \beta \sqrt{S_t m_{eff}} , \tag{1.8d} \]

where

\[ S_n = 2 Y_{eff} \sqrt{R_{eff} \delta_n} \tag{1.9a} \]
\[ S_t = 2 G_{eff} \sqrt{R_{eff} \delta_n} \tag{1.9b} \]
\[ \beta = \frac{\ln(c_r)}{\sqrt{\ln^2(c_r) + \pi^2}} \tag{1.9c} \]

In Eqs. (1.6) – (1.9) we used:

\[ m_{eff} = \left( \frac{1}{m_i} + \frac{1}{m_j} \right)^{-1} \tag{1.10a} \]
\[ R_{eff} = \left( \frac{1}{R_i} + \frac{1}{R_j} \right)^{-1} \tag{1.10b} \]
\[ Y_{eff} = \left( \frac{1 - \nu_i^2}{Y_i} + \frac{1 - \nu_j^2}{Y_j} \right)^{-1} \tag{1.10c} \]
\[ G_{eff} = \left( \frac{2(2 + \nu_i)(1 - \nu_i)}{Y_i} + \frac{2(2 + \nu_j)(1 - \nu_j)}{Y_j} \right)^{-1} , \tag{1.10d} \]

where \( i \) and \( j \) are indexes of colliding bodies.

In the final part of this section, conditions imposed on single- and multi-step models in order to satisfy Coulomb friction postulates are presented. Two friction regimes (static and kinetic) are distinguished. In the former regime, following inequality has to be satisfied:

\[ k_t \delta_t \leq \mu F_n, \tag{1.11} \]
where $\mu$ is a coefficient of friction between two colliding bodies. Inequality (1.11) involves only elastic part of friction force. Viscous part was neglected in (1.11) since it is multiplied by the magnitude of tangential velocity, which should be zero in static regime.

Kinetic friction occurs when (1.11) is not satisfied. In both contact history models (one- and multi-stepped) viscous part of friction force is clamped to 0. The reason for that is to keep Coulomb’s limit strict and independent of velocity.

In case of one-step history model the projection of contact force on Coulomb’s cone is given in (1.12).

$$F_t = \begin{cases} \mu F_n, & k_t \delta_t > \mu F_n, \\ F_t, & \text{otherwise,} \end{cases}$$  

(1.12)

where $\mu$ is friction coefficient. Viscous part of $F_t$ is set to zero when $k_t \delta_t > \mu F_n$ and, as said previously, it should also be equal to zero when $k_t \delta_t \leq \mu F_n$.

When it comes to the multi-step history model, not only the contact force is projected on the Coulomb’s cone, but the current tangential displacement is shrunk, as well.

$$F_t = \begin{cases} \frac{\mu F_n}{k_t} \delta_t, & k_t \delta_t > \mu F_n \\ F_t, & \text{otherwise} \end{cases}$$  

(1.13)

$$\delta_t = \begin{cases} \frac{\mu F_n}{k_t} \delta_t, & k_t \delta_t > \mu F_n \\ \delta_t, & \text{otherwise} \end{cases}$$  

(1.14)

Similarly to the one-step model, viscous part is clamped to 0 in kinetic friction regime. When $k_t \delta_t \leq \mu F_n$, so in static friction case, tangential velocity should be zero.

### 1.2 Complementary Based Discrete Element Method

In this section we presented method which, unlike DEM-P described in Section 1.1, models simulated bodies as rigid and impose a non-penetration requirement during their collision [5, 6].
This method, called DEM-C, handles friction and contact issues via imposing complementarity conditions on the mechanical system, see Eq. (1.15c). Whole differential variational inequality problem was stated in (1.15).

\[
\dot{q} = L(\epsilon)v \\
M\dot{v} = F(q, v, t) + G\dot{\lambda} + D\dot{\gamma}
\]

\[
g(q, t) = 0
\]

\[
0 \leq \Phi_i(q, t) \perp \gamma_{i,n} \geq 0
\]

\[
0 \leq \sqrt{v_{i,u}^2 + v_{i,w}^2} \perp \mu_i\gamma_{i,u} - \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2} \geq 0, \quad i = 1, \ldots, n_c
\]

\[
v_{i,\tau} \circ \gamma_{i,\tau} = -|v_{i,\tau}| |\gamma_{i,\tau}|,
\]

where \(v_{i,\tau} = [v_{i,u}, v_{i,w}]^T\) and \(\gamma_{i,\tau} = [\gamma_{i,u}, \gamma_{i,w}]^T\). Equation (1.15a) shows mapping of velocity vector, \(v \in \mathbb{R}^{6n_b}\), where angular velocities were expressed in the local coordinates into vector of time derivatives of generalized coordinates, where orientations were expressed by using Euler Parameters, \(q \in \mathbb{R}^{7n_b}\), see Eqs. (1.16) and (1.17).

\[
q = [r_1^T, \epsilon_1^T, \ldots, r_{n_b}^T, \epsilon_{n_b}^T]^T \in \mathbb{R}^{7n_b \times 1}
\]

\[
v = [\dot{r}_1^T, \dot{\epsilon}_1^T, \ldots, \dot{r}_{n_b}^T, \dot{\epsilon}_{n_b}^T]^T \in \mathbb{R}^{6n_b \times 1}
\]

Hence, \(L\) has to be a matrix having form shown in Eq. (1.18). It consists of identity matrices and matrices \(B_i = B(\epsilon_i)\), which transform vectors \(\omega_i\) into vectors \(\dot{q}_i\), where \(i = 1, \ldots, n_b\) [7].
\[
L = \begin{bmatrix}
I_{3 \times 3} \\
\vdots \\
I_{3 \times 3}
\end{bmatrix}
B_1 
\cdots 
B_{n_b}
\in \mathbb{R}^{7n_b \times 6n_b}
\tag{1.18}
\]

\[
B(\epsilon) = 0.5 \begin{bmatrix}
-\epsilon_1 & -\epsilon_2 & -\epsilon_3 \\
\epsilon_0 & -\epsilon_3 & \epsilon_2 \\
\epsilon_3 & \epsilon_0 & -\epsilon_1 \\
-\epsilon_2 & \epsilon_1 & \epsilon_0
\end{bmatrix}
\in \mathbb{R}^{4 \times 3}
\tag{1.19}
\]

Equation (1.15b) is a Newton’s second law of motion. \( M \) is a constant mass matrix,

\[
M = \begin{bmatrix}
m_1 I_{3 \times 3} \\
J_1 \\
\vdots \\
m_{n_b} I_{3 \times 3}
\end{bmatrix}
\in \mathbb{R}^{6n_b \times 6n_b},
\]

where \( m_i \) is a mass and \( J_i \) is a moment of inertia expressed in local coordinate system of \( i \)-th body. \( F(q, v, t) \in \mathbb{R}^{6n_b} \) is a vector of applied forces and torques. Terms \( G\dot{\lambda} \) and \( D\dot{\gamma} \) represent reaction forces coming from bi- and unilateral constraints, respectively.

Matrix \( G \) can be defined as \( G = L^T g_q^T \in \mathbb{R}^{6n_b \times n_q} \), where \( g_q \) is a Jacobi matrix of bilateral constrains, and definition of \( L \) was presented in Eq. (1.18). \( G \) was also derived in Eq. (1.20).

\[
\dot{g}(\dot{q}, q, t) = g_i(q, t) + g_q \dot{q}
\tag{1.20a}
\]

\[
\dot{g}(v, q, t) = g_i(q, t) + g_q L(q)v = g_i(q, t) + G^T v
\tag{1.20b}
\]
Figure 1.2: Bodies A and B in contact; a local reference frame \( \{ \mathbf{n}_i, \mathbf{u}_i, \mathbf{w}_i \} \) is generated at the contact point based on contact detection information. The contact point is located in the co-centric and principal reference frames via the \( s_{i,A} \) and \( s_{i,B} \) constant vectors. Original picture and caption were taken from [8]; the picture was modified, before being presented it in this work.

Matrix \( \mathbf{D} \), on the other hand, maps Lagrange multipliers associated with active unilateral constraints into forces and torques represented in global coordinate system.

\[
\mathbf{D} = \left[ \mathbf{D}_1, \ldots, \mathbf{D}_{n_c} \right] \in \mathbb{R}^{6n_b \times 3n_c}, \tag{1.21}
\]

where

\[
\mathbf{D}_i = \left[ \ldots, 0_{3 \times 3}, -\mathbf{A}_i^T, \mathbf{A}_i^T \mathbf{A}_A \mathbf{s}_{i,A}, 0_{3 \times 3}, \ldots, 0_{3 \times 3}, \mathbf{A}_i^T, -\mathbf{A}_i^T \mathbf{A}_B \mathbf{s}_{i,B}, 0_{3 \times 3}, \ldots \right]^T \tag{1.22}
\]

In Equation (1.22) matrices of transformation \( \mathbf{D}_i \in \mathbb{R}^{6n_b \times 3} \) corresponding to \( i \)-th contact were presented (colliding bodies have indexes \( A \) and \( B \)). Columns of matrix \( \mathbf{A}_i \), where \( i \) is an index of contact, are unit vectors of a local reference frame \( \mathbf{A}_i = [\mathbf{n}_i, \mathbf{u}_i, \mathbf{w}_i] \) generated at contact point \( i \). Matrix \( \mathbf{A}_A \), where \( A \) is an index of a colliding body, is a local reference.
frame determining orientation of body $A$. Vector $s_{i,A}$ points from center of mass of body $A$ to contact point $i$. Quantities $A_i$, $A_A$ and $s_{i,A}$ were visualized in Fig. 1.2.

\[ \hat{\lambda} \in \mathbb{R}^{n_B} \text{ and } \hat{\gamma} \in \mathbb{R}^{3n_c} \text{ are vectors of Lagrange multipliers. Length of } \hat{\lambda} \text{ is equal to the number of all degrees of freedom taken from the system by bilateral constraints, while vector } \hat{\lambda} \text{ associates three Lagrange multipliers to each active contact, see Eq. (1.23).} \]

\[
\hat{\gamma} = \left[ \begin{array}{c} \hat{\gamma}_1 \\ \vdots \\ \hat{\gamma}_{n_c} \end{array} \right], \quad \hat{\gamma}_i = \left[ \begin{array}{c} \hat{\gamma}_{i,n} \\ \hat{\gamma}_{i,u} \\ \hat{\gamma}_{i,w} \end{array} \right], \quad i = 1, \ldots, n_c
\] (1.23)

Equations (1.15d) – (1.15f) represent contact and friction model of colliding bodies. Based on inequalities and complementarity conditions (1.15d) we can distinguish if bodies collide (or not), and hence, if normal reaction force occurs between them. Namely, if function $\Phi$ (which can be interpreted as a distance between bodies) is positive, then bodies do not collide and the magnitude of reaction force is zero, $\hat{\gamma}_n = 0$. In case of $\Phi = 0$, bodies are in contact and $\hat{\gamma}_n \geq 0$. We consider cases where $\Phi_i = 0$, thus $i \in A = \{ 1, \ldots, n_c \}$.

Complementarity conditions in (1.15e) introduce Coulomb’s cone limit to our model. Namely, if there is no slip between colliding bodies ($|v_{i,\tau}| = 0$), then friction force is unknown and limited by Coulomb’s limit, i. e. $|\gamma_{i,\tau}| \leq \mu_i \gamma_{i,n}$. Otherwise, if bodies slide on one another, contact force vector has to lay on a Coulomb’s cone surface, $|\gamma_{i,\tau}| = \mu_i \gamma_{i,n}$. Equation (1.15f) requires vectors of relative tangential velocity and friction force to have the same direction, but opposite senses.

Set of differential variational inequalities (1.15) can be brought to a quadratic optimization problem with conical constraints via discretization and introduction of stability, compensation and relaxation terms. Consider a set of equations and inequalities presented in (1.24).

\[
q^{(l+1)} = q^{(l)} + \Delta t \ L \ v^{(l+1)}
\] (1.24a)

\[
M \ (v^{(l+1)} - v^{(l)}) = \Delta t \ F^{(l)} + G^{(l)} \lambda^{(l+1)} + D^{(l)} \gamma^{(l+1)}
\] (1.24b)
\[
\frac{1}{\Delta t} g^{(l)} + g^{(l)}_t + (G^{(l)})^T v^{(l+1)} = 0
\]  
(1.24c)

\[
\begin{align*}
\text{stabilization term} \\
0 \leq \frac{1}{\Delta t} \Phi^{(l)}_i + v^{(l+1)}_{i,n} - \mu_i \sqrt{(v^{(l+1)}_{i,u})^2 + (v^{(l+1)}_{i,w})^2} \perp \gamma^{(l+1)}_{i,n} & \geq 0 \\
\text{relaxation term} \\
0 \leq \sqrt{(v^{(l+1)}_{i,u})^2 + (v^{(l+1)}_{i,w})^2} \perp \mu_i \gamma^{(l+1)}_{i,n} - \sqrt{(\gamma^{(l+1)}_{i,u})^2 + (\gamma^{(l+1)}_{i,w})^2} & \geq 0, \quad i \in \{1, \ldots, n_c\}
\end{align*}
\]  
(1.24d)

where \( \lambda = \Delta t \hat{\lambda} \) and \( \gamma = \Delta t \hat{\gamma} \).

Two modifications had to be made to discretized Eqs. (1.15) in order to bring it to from shown in (1.24):

1. First of all, Eq. (1.24c) is not a discretized Eq. (1.15c). It is rather its first time derivative discretized. However, a stabilization term \( \frac{1}{\Delta t} g^{(l)} \) is present in Eq. (1.24c), thus the attempt to satisfy Eq. (1.15c) on velocities’ and positions’ level was taken.

2. Gap function from inequality (1.15d) was approximated by \( \Phi^{(l+1)}_i \approx \Phi^{(l)}_i + \Delta t v^{(l+1)}_{i,n} \). Additionally, an inequality on the left was relaxed by adding term \( \Delta t \left( \mu_i \gamma^{(l+1)}_{i,n} - \sqrt{(\gamma^{(l+1)}_{i,u})^2 + (\gamma^{(l+1)}_{i,w})^2} \right) \). With this relaxation term, it is possible to bring the discretized differential variational inequality problem (1.24) to equivalent cone complementarity problem. It can also be shown that the relaxation will not impact the solution of problem in its original formulation when the step size goes to zero [9].

Set of discretized equations and inequalities (1.24c) - (1.24f) can be brought to conically constrained quadratic optimization problem in following form (for details see [8]):

\[
\begin{align*}
\arg\min_{\zeta} & \quad \frac{1}{2} \zeta^T N \zeta + r^T \zeta \\
\text{s. t.} & \quad \zeta_i \in \Upsilon_i, \quad i = 1, \ldots, n_c + n_{bi}
\end{align*}
\]  
(1.25)
where $\zeta_i$'s represent Lagrange multipliers associated with either bi- or unilateral constraints; $\Upsilon_i = \mathbb{R}$ for every $\lambda_i$, or it is a Coulomb's friction cone associated with $i$-th active bilateral constraint.

The moment (1.25) is solved for $\zeta$, Lagrange multipliers $\lambda$ and $\gamma$ are known. Hence, velocities and positions in $(l+1)$-th (current) time step can be obtained from Eqs. (1.24a) and (1.24b).
2 MODELING DYNAMICS SYSTEMS USING CHRONO

Chrono is an open source software infrastructure used to investigate the dynamics; i.e., time evolution, of multibody systems governed by very large sets of ordinary differential equations and/or differential algebraic equations and/or partial differential equations [10, 11]. From a user perspective, Chrono rests on five foundation components that provide the following basic functionality: equation formulation, equation solution, collision detection, domain decomposition for parallel computing, and pre/post-processing, see Fig. 2.1.

The first foundation component, called “Equation Formulation”, supports general purpose modeling for the time evolution (dynamics) of large systems of rigid and flexible bodies and for fluid-solid interaction problems. This translates into the ability to generate ordinary differential equations, differential algebraic equations, or partial differential equations associated with the problem modeled. The second component, called “Equation Solution”, provides algorithmic support needed to numerically solve the resulting equations of motion (EOM). This is the component that implements, for instance, the functionality to solve a large, sparse linear system of equations efficiently using parallel computing. Proximity computation support, essential for collision detection and computation of short and medium range interaction forces, is provided by the third foundation component. The fourth component enables the partitioning and farming out of very large dynamics problems for parallel execution on supercomputer architectures using the Message Passing Interface (MPI) paradigm [12]. The fifth component provides pre- and post-processing support. Whenever a piece of functionality is added to Chrono, it finds a home in one of these five components. It either enriches the physics modeled by Chrono, improves the robustness, efficiency, or accuracy of the numerical solution, helps the pre/post processing, etc. Finally, since physics-based simulation is computationally demanding, Chrono draws on high performance computing at each stage of the model $\rightarrow$ simulate $\rightarrow$ visualize process.

Chrono’s strength lies in its ability to simulate the dynamics of large multibody systems. These systems can be made up of rigid and compliant bodies, which, in the most general
Figure 2.1: An abstraction of Chrono architecture, user perspective. Vertical applications draw support from an underlying set of five foundation components responsible for equation formulation, equation solution, collision detection, HPC support, and pre/post processing tasks.

case, may interact with fluid. Support for modeling and simulating fluid-solid interaction problems is provided by Chrono::Fluid. Discipline-specific support is also provided for ground vehicle modeling and simulation (Chrono::Vehicle), soil/terrain modeling and simulation (Chrono::Terramechanics), etc. Note that these domains, or discipline specific views, also called verticals, do not map one-to-one into the software structure of Chrono shown in Fig. 2.2, which provides a developer perspective of the actual software infrastructure. However, these domain specific views are convenient to explain the family of practical applications that can be modeled and solved with Chrono through predefined templates that ease the modeling burden. For instance, Chrono::Vehicle provides templates for vehicle suspension, steering line, basic powertrain, rigid road profile, etc., much like ADAMS/Car does [13].

Unlike the block diagram in Fig. 2.1, which provides an abstract, high-level, user perspective of Chrono, Fig. 2.2 illustrates its structure from a software design vantage point. The image presents a snapshot of an evolving open source software infrastructure backed by more than 40 years of man-effort and evaluated at $2.4 million by Ohloh, a public directory of Free and Open Source Software. Chrono::Engine, the backbone of Chrono, is made up of C++ classes that implement rigid body dynamics simulation, collision detection, etc.
Figure 2.2: A developer’s perspective of the modular architecture of Chrono reflects its software design philosophy: recycle existing solutions and produce new ones that are aligned with the core competencies of the group. The main research and development is focused on the Chrono::Engine core as well as the FEM, Flex, Fluid, LinearAlgebra and HPC units.

Additional features such as finite element analysis, support for co-simulation, fluid dynamics, etc., are accessible via dynamically-linked libraries. This entire infrastructure is provided with a unitary C++ Application Programming Interface (API), which enforces a regimented way of interacting with the Chrono::Engine and the various units. The API comes in two flavors: the low level is in C++, the high level is Python-based [14], and their purpose is to separate the software implementation details from the user. For the latter, one only needs to be aware of how Chrono::PyEngine should to be used to define, for instance, a scenario such as a vehicle riding over granular soil. A collection of such Python files enables one to talk about Chrono::Flex, Chrono::Vehicle, Chrono::Fluid, etc. Building a vehicle model for instance can be done in one of two ways: by starting with an existing Chrono::Vehicle template and modifying its parameters, or by building the model from scratch and writing lines of Python script to instantiate through Chrono::PyEngine a body called ‘chassis’ using a geometry specified in an obj file, connecting this body to another body called ‘lower control arm’, and so on, thus building the model from scratch.
3 Case Study

3.1 Numerical Side of Simulations

In this section aspects of numerical side of simulations which were common to all the tests conducted on will be described. Additional information, specific to each of three tests, was presented in Sections 3.2.2.2, 3.3.2.2 and 3.4.2.2.

Simulations of three often-encountered geomechanical tests were presented in this thesis, namely: (i) cone penetration test, (ii) standard triaxial test and (iii) direct shear test. Mechanical systems were modeled with a usage of two different methods allowing for handling of friction and contact forces between colliding bodies. Since bodies were treated in a discrete fashion (position and orientation of each body was tracked) the algorithms can be classified as members of a family of Discrete Element Methods (DEM). However, the way the friction and contact forces were computed allows us to classify them as penalty and complementarity methods. Complementarity method (or DEM-C), treats bodies as rigid and requires solver to satisfy a non-penetration complementarity conditions when bodies collide. Penalty approach, allows inter-penetrations between colliding elements and puts a penalty-type condition on them. This method is called DEM-P, from “penalty”.

Both DEM-P and DEM-C can be successfully used in simulating mechanical phenomena. If calibrated correctly, simulations based on those algorithms should give the results that are close to empirical measurements and to each other. By correct calibration we meant choosing correct numerical values for parameters those two approaches can be characterized with from the numerical point of view. Correct values of parameters should provide stability of computations and model the physics sufficiently well.

Stability of calculations in DEM-P model can be ensured by choosing correct values of time step ($\Delta t$). While using DEM-C approach, combination of following parameters: time step, contact recovery speed (CRS) and Maximum Number of Iterations (MNoI) is important.
In both modeling approaches $\Delta t$ is the parameter responsible for the stability of calculations. Too large values of $\Delta t$ will make the simulations unstable, too small - will result in having very long execution time. The optimal value of $\Delta t$ can be chosen via a trial and error method.

Time steps’ values in simulations of cone penetration and standard triaxial tests [15, 16], were about 10 times larger when using DEM-C, comparing to those from simulations based on DEM-P.

In simulation of direct shear test [17], $\Delta t$ used in DEM-C approach was up to 450 times larger that in the DEM-P one. It was mainly caused by the upper limit put on the time step values in DEM-P simulations ($\Delta t = 2 \times 10^{-6}$ seconds). Such small values were dictated by the lack of relaxation of stiffness describing elastic parts of contact forces (Young’s modulus of each body was equal to, $50 \times 10^9$ Pa). In simulations of standard triaxial or cone penetration tests Young’s modulus were given smaller than in reality values, what allowed for having larger time steps.

Contact recovery speed (CRS) is a parameter used only in DEM-C-based simulations. As its name indicates, this parameter puts the upped limit on the normal component of velocities two colliding bodies rebound from each other with. Even though the complementarity approach models bodies as they were rigid, at the beginning of each time step, colliding bodies can actually overlap each other, assigning a penetration depth to such contact. In certain cases, normal components of velocities two bodies will rebound off each other with is equal to the penetration depth divided by the time step. If value of this component exceeds the value of a particular upper limit (called contact recovery speed) it will be simply clamped to this limit’s value. In other words, CRS provides stability to simulations and allows for having larger values of $\Delta t$. Thus, it additionally makes the execution time of simulations shorter.

In DEM-C method user can decide on the Maximum Number of Iterations (MNoI) done in every time step. During the iterative process, normal and tangential components of contact forces are being calculated. MNoI depends on a type of the test being simulated. In simulation
of cone penetration test (CPT) 50 iterations per time step were enough to make results reasonable. Calculations with MNoI set up to 500 gave satisfactory results concerning direct shear tests. Simulations of standard triaxial test required up to 2500 iterations per time step to make calculation not only stable but also giving results correct from the physical point of view.

Values of the above-described parameters used in simulations of cone penetration, standard triaxial and direct shear tests were presented in Tabs. 3.8, 3.24 and 3.32.

\section*{3.2 Cone Penetration Test}

\subsection*{3.2.1 Laboratory Experiments}

\subsubsection*{3.2.1.1 Overview}

Detailed report on the laboratory cone penetration test is available in [18]. Aspects of the experiment which needed to be considered during the numerical modeling were described in this section. Mechanical and geometrical parameters of bodies used in the empirical tests were provided. Additionally, an impact of the experimental apparatus on the results was briefly described.

The laboratory tests were conducted on using two cylindrical containers with diameters of 4 and 6 in (10.16 and 15.24 cm, respectively). They were 11.64-cm-high and fully filled out with a granular material consisting of imperfect spheres (see Tab. 3.1). Those imperfect spheres were made of glass and could be modeled as ellipsoids with diameters from the following normal distribution: \( N(2.84, 0.0834) \) mm (Tab. 3.2). Following the standardized procedures (ASTM D5254) specimens were placed in containers via ways which allowed them for obtaining two different densities and void ratios (Tab. 3.3).

Cones of two different geometrical dimensions were dropped on such prepared granular samples. In first scenario, cone had the altitude of \( L_{30\degree} = 34.36 \) mm, base’s diameter equal to \( W_{30\degree} = 9.21 \) mm and the apex angle of 30°. The other cone was 22.10-mm-high (\( L_{60\degree} \)),
Figure 3.1: Schematic diagram of a cone drop experiment. The drop height (H), cone altitude (L) and width (W) are illustrated in the picture.

Table 3.1: Geometrical dimensions of containers used in experiments.

<table>
<thead>
<tr>
<th>Containers</th>
<th>Diameter [in (cm)]</th>
<th>Height [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4 (10.16)</td>
<td>11.64</td>
</tr>
<tr>
<td></td>
<td>6 (15.24)</td>
<td></td>
</tr>
</tbody>
</table>

diameter of its base ($W_{60^\circ}$) was 19.86-mm-wide and it had the apex angle of $60^\circ$. Cones were made of brass steel of following mechanical parameters: Young’s modulus, $Y = 193 \cdot 10^9$ Pa and Poisson’s ratio from the following range: $\nu \in [0.3, 0.31]$ (Table 3.4).

Cones were attached, using a special connector, to a Linear Variable Differential Transformer (LVDT) - apparatus which allowed for monitoring cone’s vertical position while it was falling and penetrating the granular media. Cones, $30^\circ$ and $60^\circ$ in apex angle, together with the LVDT connector had mass of 141.1 g and 135.7 g, respectively (Table 3.4).

Besides attaching the additional mass to falling bodies, the LVDT apparatus affected the experimental results in two more ways. Firstly, it put a kinematic constraint on cones’ trajectories. Namely, cones’ axis of symmetry had to remain vertical at every time instant of its motion. It was caused by a vertical rod connecting cones with the rest of the machinery; the rod was shown in Fig. 3.2a. Secondly, there was a friction force acting between the before-mentioned rod and its track. Value of this friction force was measured during all the experiments conducted on, resulting in 0.03 N, what decreased the cones’ downward acceleration by $2.21 \frac{m}{s^2}$. 
(a) Cone, with $30^\circ$ in apex angle, attached to Linear Variable Differential Transformer (LVDT) connector. Rod, which put a kinematic constraint on cone’s motion, as well as rod’s track can also be seen in the picture. (b) One of two containers used in the experiment. Apparatus used in measuring cone displacement is placed above it. Picture was taken right before one of the cone penetration tests was conducted on.

Figure 3.2: Pictures of the apparatus used in the experiment.

Table 3.2: Geometrical dimensions and material of the particles used in the experiments.

<table>
<thead>
<tr>
<th>Granular material</th>
<th>Shape</th>
<th>Diameters distribution [mm]</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ellipsoids</td>
<td>N(2.84, 0.0834)</td>
<td>Glass</td>
<td></td>
</tr>
</tbody>
</table>

The last information needed to be taken into account while setting up the simulations was a height cones were dropped from (the height was relative to the surface of the settled specimen). In a static cone penetration test, cones were placed right above the surface of granular material (zero drop height). In the dynamic loading, cones were dropped from two heights above the surface of the granular material. First height was equal to the dropped cone’s altitude ($L_{30^\circ} = 34.36 \text{ mm}$, $L_{60^\circ} = 22.10 \text{ mm}$), the other one was equal to its half ($\frac{1}{2}L_{30^\circ} = 17.18 \text{ mm}$, $\frac{1}{2}L_{60^\circ} = 11.05 \text{ mm}$). Heights at which cones were placed before they were dropped:
1. Zero drop height; flush with the granular material’s surface

2. Half of cone’s altitude; \( \frac{1}{2} L_{30^\circ} = 17.18 \) mm, \( \frac{1}{2} L_{60^\circ} = 11.05 \) mm,

3. The altitude of the cones; \( L_{30^\circ} = 34.36 \) mm, \( L_{60^\circ} = 22.10 \) mm,

(a) Cones with 60\(^\circ\) and 30\(^\circ\) in their apex angles.

(b) Cones with attached LVDT connectors.

Figure 3.3: Pictures of cones used in experiments.

Table 3.3: Densities and void ratios of settled specimens used in empirical tests.

<table>
<thead>
<tr>
<th></th>
<th>Density ( \text{kg/m}^3 )</th>
<th>Void Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose Case</td>
<td>1504.32</td>
<td>0.66</td>
</tr>
<tr>
<td>Dense Case</td>
<td>1630.35</td>
<td>0.53</td>
</tr>
</tbody>
</table>

Table 3.4: Geometrical dimensions and mechanical parameters of cones used in laboratory tests.
*Mass of cones together with the LVDT connector.

<table>
<thead>
<tr>
<th></th>
<th>Apex angle</th>
<th>Height [mm]</th>
<th>Base’s Diameter [mm]</th>
<th>( Y [\text{Pa}] )</th>
<th>( \nu )</th>
<th>mass* [g]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cones</td>
<td>30(^\circ)</td>
<td>34.36</td>
<td>9.21</td>
<td>( 193 \cdot 10^9 )</td>
<td>0.3 ( \div ) 0.31</td>
<td>141.1</td>
</tr>
<tr>
<td></td>
<td>60(^\circ)</td>
<td>22.10</td>
<td>19.86</td>
<td></td>
<td></td>
<td>135.7</td>
</tr>
</tbody>
</table>
3.2.1.2 Results

Below, the experimental results presented in [18] were shown.

Figure 3.4: Depth/height vs. time plots of cone $30^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.

Figure 3.5: Depth/height vs. time plots of cone $30^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed densely.
Figure 3.6: Depth/height vs. time plots of cone 30° in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.7: Depth/height vs. time plots of cone 30° in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
Figure 3.8: Depth/height vs. time plots of cone $60^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.

Figure 3.9: Depth/height vs. time plots of cone $60^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed densely.
Figure 3.10: Depth/height vs. time plots of cone 60° in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.11: Depth/height vs. time plots of cone 60° in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
3.2.2 Numerical Simulations

3.2.2.1 Physical Side of Simulations

Simulations were divided into two stages. During the first one (settling stage), granular material was poured into a container and was allowed to gain its equilibrium state (see plots of specimen’s kinetic energy in Fig. 3.12). Second stage (cone penetration stage) was about placing cone right above the surface of the settled granular material and dropping it with an initial vertical velocity equal to $\sqrt{2(g-a)H}$, where:

- $g$ – Earth’s gravity,
- $a$ – average upward acceleration caused by the friction force acting between the LVDT apparatus’ rod and its track; $a = 2.21 m/s^2$
- $H$ – initial height cones were dropped from ($H \in \{0, \frac{1}{2}L_i, L_i\}, i \in \{30^\circ, 60^\circ\}$)

Containers with diameters of 4 and 6 inches were filled out with granular material consisting of perfect spheres. Particles, each of 2.84 mm in diameter, were made of glass and had following mechanical parameters: density, $\rho = 2500 \ kg/m^3$; Young’s modulus, $Y = 10^8 \ Pa$ (value lower
Table 3.5: Values of particles’ mechanical parameters used in the simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\rho$ [kg/m$^3$]</th>
<th>$Y$ [Pa]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granular material</td>
<td>Glass</td>
<td>2500</td>
<td>$10^8$</td>
</tr>
</tbody>
</table>

Table 3.6: Values of cones’ mechanical parameters used in simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>Apex angle</th>
<th>$Y$ [Pa]</th>
<th>$\nu$</th>
<th>mass* [g]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cones</td>
<td>Brass</td>
<td>30$^\circ$</td>
<td>193 $\cdot$ $10^9$</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>Steel</td>
<td>60$^\circ$</td>
<td>135.7</td>
<td></td>
</tr>
</tbody>
</table>

than in reality for stability reasons); Poisson’s ratio, $\nu = 0.3$. Coefficient of restitution between colliding particles ($c_{r,p-p}$) was set to 0.658 [19]. Walls of the container were massless and had mechanical parameters of the same values as particles.

A few words of explanation are in order concerning the values of friction coefficients between particles ($\mu_{\text{particle-particle}}$, $\mu_{p-p}$) and between particles and containers’ walls ($\mu_{\text{particle-wall}}$, $\mu_{p-w}$). Values of those parameters played significant role in obtaining looser and denser packings of settled granular material. Namely, when the coefficients of friction were set to 0.7, settled sample had density similar to the one from the empirical loose case. Packing seen in the experimental dense case scenario was achieved after a settling stage simulation with frictionless walls and particles ($\mu_{p-p} = \mu_{p-w} = 0.0$). In the second part of the simulation (cone penetration stage), two before-mentioned friction coefficients together with $\mu_{\text{particle-cone}}$ ($\mu_{p-c}$) were set to 0.7. Analysis of the friction coefficients’ impact on the results was described in Sections 3.2.3.1 and 3.2.3.2. Values of friction coefficients match ones found in engineering tables [20].

Cones used in the simulations were given the geometrical dimensions and masses presented in Tab. 3.4. They were made of brass steel and were given the following parameters: Young’s modulus, $Y = 193 \cdot 10^9$ Pa; Poisson’s ratio, $\nu = 0.3$. Coefficients of restitution and friction between the steel cone and glass beads were equal to: $c_{r,p-c} = 0.597$ [19] and $\mu_{p-c} = 0.7$ [20], respectively.
Table 3.7: Values of mechanical parameters describing contacts used in simulations.

<table>
<thead>
<tr>
<th></th>
<th>$\mu_{p-p}$</th>
<th>$\mu_{p-w}$</th>
<th>$c_{r,p-p}$</th>
<th>$c_{r,p-w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loose Case</td>
<td>0.7</td>
<td>0.7</td>
<td>0.658</td>
<td>0.658</td>
</tr>
<tr>
<td>Dense Case</td>
<td>0.0</td>
<td>0.0</td>
<td>0.658</td>
<td>0.658</td>
</tr>
</tbody>
</table>

CPT Test

<table>
<thead>
<tr>
<th></th>
<th>$\mu_{p-p}$</th>
<th>$\mu_{p-w}$</th>
<th>$c_{r,p-p}$</th>
<th>$c_{r,p-w}$</th>
<th>$\mu_{p-c}$</th>
<th>$c_{r,p-c}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Both Cases</td>
<td>0.7</td>
<td>0.7</td>
<td>0.658</td>
<td>0.658</td>
<td>0.7</td>
<td>0.597</td>
</tr>
</tbody>
</table>

A kinematic constraint was put on the cones to model the impact of the rod they were attached to. With such constraint cones’ symmetry axis remained vertical at the every time instant.

3.2.2.2 Numerical Side of Cone Penetration Test Simulations

General information on numerical side of simulations was given in Section 3.1. In this section we will summarize values of numerical parameters used in simulations of cone penetration test (Tab. 3.8).

Table 3.8: Numerical parameters’ values used in simulations. *MNoI - Maximum Number of Iterations; ** CRS - Contact Recovery Speed.

<table>
<thead>
<tr>
<th>Approach</th>
<th>time step [s]</th>
<th>MNoI*</th>
<th>CRS** [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>$10^{-5}$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>DEM-C</td>
<td>$10^{-4}$</td>
<td>50</td>
<td>1.0</td>
</tr>
</tbody>
</table>
Figure 3.13: Cone penetration test - numerical setup: (a) cone placed over the settled specimen; (b) cone penetrating the granular material.
3.2.2.3 Results

In this section results obtained from the simulations were presented. They were additionally compared to the experimental data. Densities and void ratios of granular materials in their equilibrium state were summarized in Tabs. 3.9 – 3.12. Relative error between results from simulations and empirical tests varied from 1.19 % to 5.20 % concerning densities and from 3.85 % to 13.79 % when it comes to void ratios. Vertical displacements of cones as functions of time were presented in Figs. 3.14 – 3.21. Numerical results matched the experimental ones. Moreover, even though two approaches model frictional contact differently and use different sets of numerical parameters to describe physical phenomena, the outcomes from simulations based on DEM-P and DEM-C were comparable.

Table 3.9: A comparison of experimental and numerical results. Densities of samples in their equilibrium state. Container with a diameter of 4 inches.

<table>
<thead>
<tr>
<th>Densities $[\text{kg/m}^3]$</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DEM-P</td>
<td>DEM-C</td>
</tr>
<tr>
<td>Loose Case</td>
<td>1504.29</td>
<td>1449.59</td>
<td>1426.00</td>
</tr>
<tr>
<td>Dense Case</td>
<td>1630.34</td>
<td>1608.79</td>
<td>1593.69</td>
</tr>
</tbody>
</table>

Table 3.10: A comparison of experimental and numerical results. Densities of samples in their equilibrium state. Container with a diameter of 6 inches.

<table>
<thead>
<tr>
<th>Densities $[\text{kg/m}^3]$</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DEM-P</td>
<td>DEM-C</td>
</tr>
<tr>
<td>Loose Case</td>
<td>1504.32</td>
<td>1462.70</td>
<td>1433.39</td>
</tr>
<tr>
<td>Dense Case</td>
<td>1630.35</td>
<td>1610.93</td>
<td>1601.22</td>
</tr>
</tbody>
</table>
Figure 3.14: Height/depth vs. time plots of cone with 30° in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.

Table 3.11: A comparison of experimental and numerical results. Void ratios of samples in their equilibrium state. Container with a diameter of 4 inches.

<table>
<thead>
<tr>
<th>Void Ratios</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DEM-P</td>
<td>DEM-C</td>
</tr>
<tr>
<td>Loose Case</td>
<td>0.66</td>
<td>0.72</td>
<td>0.75</td>
</tr>
<tr>
<td>Dense Case</td>
<td>0.53</td>
<td>0.55</td>
<td>0.57</td>
</tr>
</tbody>
</table>
Figure 3.15: Height/depth vs. time plots of cone with 30° in apex angle. Container with a 4-inches-wide diameter. Granular material packed densely.

Table 3.12: A comparison of experimental and numerical results. Void ratios of samples in their equilibrium state. Container with a diameter of 6 inches.

<table>
<thead>
<tr>
<th>Void Ratios</th>
<th>Experiment</th>
<th>Simulation</th>
<th>Relative Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>DEM-P</td>
<td>DEM-C</td>
</tr>
<tr>
<td>Loose Case</td>
<td>0.66</td>
<td>0.71</td>
<td>0.74</td>
</tr>
<tr>
<td>Dense Case</td>
<td>0.53</td>
<td>0.55</td>
<td>0.56</td>
</tr>
</tbody>
</table>
Figure 3.16: Height/depth vs. time plots of cone with $30^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.17: Height/depth vs. time plots of cone with $30^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
Figure 3.18: Height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.

Figure 3.19: Height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed densely.
Figure 3.20: Height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.21: Height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
3.2.2.4 Performance analysis

Execution time of cone penetration test simulation will be discussed in this section. As mentioned previously, simulations consisted of two parts – settling] and cone penetration stages. In the former one, after pouring granular material into the container it was allowed to gain its equilibrium state. Settling stage last 1.0 second of simulated time, despite the fact that the equilibrium state was gained earlier (around 0.5 of the second; see Fig. 3.12). In cone penetration stage, cones were placed right above the specimen’s surface and dropped with certain initial velocity. This stage took 0.4 seconds of time simulated.

Performance of simulations based on penalty and complementarity approaches was compared, showing that the execution times of simulations based on DEM-C were about 1.6 times longer. All the simulations were run using 8 threads of Intel ES-2650 v3 @ 2.30 Ghz. Results were summarized in Tabs. 3.13 – 3.16.


<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>3 h 14 min</td>
<td>1.0</td>
<td>1.54</td>
</tr>
<tr>
<td>DEM-C</td>
<td>5 h 03 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Penetrometer Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>1 h 21 min</td>
<td>0.4</td>
<td>1.64</td>
</tr>
<tr>
<td>DEM-C</td>
<td>2 h 13 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Whole simulation</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>4 h 36 min</td>
<td>1.4</td>
<td>1.56</td>
</tr>
<tr>
<td>DEM-C</td>
<td>7 h 16 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3.14: A comparison of simulations execution time. Container with a 4-in-wide diameter. Dense packing. Number of bodies 53296.

<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>3 h 33 min</td>
<td>1.0</td>
<td>1.67</td>
</tr>
<tr>
<td>DEM-C</td>
<td>5 h 55 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Penetrometer Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>1 h 27 min</td>
<td>0.4</td>
<td>1.76</td>
</tr>
<tr>
<td>DEM-C</td>
<td>2 h 32 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Whole simulation</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>5 h 00 min</td>
<td>1.4</td>
<td>1.69</td>
</tr>
<tr>
<td>DEM-C</td>
<td>8 h 27 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>7 h 06 min</td>
<td>1.0</td>
<td>1.46</td>
</tr>
<tr>
<td>DEM-C</td>
<td>10 h 23 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
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<th>Penetrometer Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>4 h 12 min</td>
<td>0.4</td>
<td>1.78</td>
</tr>
<tr>
<td>DEM-C</td>
<td>7 h 29 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Whole simulation</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$T_{DEM-C}^{exec}/T_{DEM-P}^{exec}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>11 h 18 min</td>
<td>1.4</td>
<td>1.58</td>
</tr>
<tr>
<td>DEM-C</td>
<td>17 h 52 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3.16: A comparison of simulations execution time. Container with a 6-in-wide diameter. Dense packing. Number of bodies 120860.

<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>7 h 28 min</td>
<td>1.0</td>
<td>1.44</td>
</tr>
<tr>
<td>DEM-C</td>
<td>10 h 47 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Penetrometer Stage</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>4 h 42 min</td>
<td>0.4</td>
<td>1.71</td>
</tr>
<tr>
<td>DEM-C</td>
<td>8 h 02 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Whole simulation</th>
<th>Execution Time ($T_{exec}$)</th>
<th>Simulation time [s]</th>
<th>$\frac{T_{DEM-C}}{T_{DEM-P}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>12 h 10 min</td>
<td>1.4</td>
<td>1.55</td>
</tr>
<tr>
<td>DEM-C</td>
<td>18 h 49 min</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.2.3 Additional Analyses

3.2.3.1 Impact of the $\mu_{p-p}$ on the results

Simulations of cone penetration test were sensitive to values of inter-particle coefficient of friction ($\mu_{p-p}$). Naturally, granular material with larger values of this parameter was able to stop the falling cone earlier. It is worthy to mention that the impact of $\mu_{p-c}$ (friction coefficient between beads and cone) on the results is very little (see Section 3.2.3.2).

To understand how sensitive simulations were to the value of $\mu_{p-p}$, cone penetration stage was run for a couple of different values of this parameter, $\mu_{p-p} \in \{0.4, 0.5, 0.6, 0.7\}$. In every simulation, friction coefficient between cone and particles ($\mu_{p-c}$) was set to 0.7. Values of other numerical and mechanical parameters can be found in Tabs. 3.5 – 3.7.

Presented plots consist of curves related to $\mu_{p-p} = 0.5$ and $\mu_{p-p} = 0.7$ only, see Figs. 3.22 – 3.26. Curves corresponding to $\mu_{p-p} = 0.4$ and $\mu_{p-p} = 0.6$ were not shown there, because this would make the plots unreadable.

The analysis showed that for the larger values of $\mu_{p-p}$, cones penetrated the granular material lesser. If shown, curve corresponding to $\mu_{p-p} = 0.6$ would be located between two curves presented on the plots. Cone’s displacement, related to $\mu_{p-p} = 0.4$, was located beneath all the curves (this curve can actually be found in Section 3.2.3.2 where plots with $\mu_{p-p} = 0.4$ were showed).

It was observed that the difference between curves obtained for different values of $\mu_{p-p}$ is larger in case of simulations with granular material packed loosely. Simulations with granular material packed densely were less sensitive to values of this parameter.
Figure 3.22: Impact of $\mu_{p,c}$ on hight/depth vs. time plots of cone with $30^\circ$ in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.

Figure 3.23: Impact of $\mu_{p,c}$ on hight/depth vs. time plots of cone with $30^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.
Figure 3.24: Impact of $\mu_{p,c}$ on height/depth vs. time plots of cone with $30^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.

Figure 3.25: Impact of $\mu_{p,c}$ on height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.
Figure 3.26: Impact of $\mu_{pc}$ on height/depth vs. time plots of cone with $60^\circ$ in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
3.2.3.2 Impact of the $\mu_{\text{particle-cone}}$ on the results

In this section, impact of the values of friction coefficient between the granular matter and cones ($\mu_{p-c}$) on the results was presented. We expected cones being stopped earlier when values of analyzed parameter were larger. It turned out that $\mu_{p-c}$ had a very little influence on the simulation results.

Cone penetration part of the simulation was run for cones with $\mu_{p-c} \in \{0.5, 0.6, 0.7\}$. The inter-particle coefficient of friction was set to 0.4 in every simulation. Values of the rest of mechanical and numerical parameters can be found in Tabs. from 3.5 to 3.7. Vertical displacements of cones were shown in Figs. 3.27 – 3.31. As mentioned above, $\mu_{p-c}$ had small impact on the outcomes.

Figure 3.27: Impact of $\mu_{p-c}$ on height/depth vs. time plots of cone with 30° in apex angle. Container with a 4-inches-wide diameter. Granular material packed loosely.
Figure 3.28: Impact of $\mu_{p,c}$ on height/depth vs. time plots of cone with 30° in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.29: Impact of $\mu_{p,c}$ on height/depth vs. time plots of cone with 30° in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
Figure 3.30: Impact of $\mu_{pc}$ on height/depth vs. time plots of cone with 60° in apex angle. Container with a 6-inches-wide diameter. Granular material packed loosely.

Figure 3.31: Impact of $\mu_{pc}$ on height/depth vs. time plots of cone with 60° in apex angle. Container with a 6-inches-wide diameter. Granular material packed densely.
3.2.3.3 Impact of double sphere’s longitudinal dimension

In this section results of cone penetration test for the case when granular material consisted of “double-spheres” were presented. A double-sphere is defined as a body consisting of two spheres of equal diameters connected to each other. Its longitudinal dimension $L$ is defined as $md$, where

$m$ – a constant real number from the range of $[1.0, 2.0]$;

d – a diameter of one of the spheres.

Dimensions of a double-sphere were shown on its cross-sectional view (Fig. 3.32). A couple of examples of double-spheres – for different values of $m$ – were shown in Fig. 3.33.

Volume ($V$), radii of gyration ($i_{xx}, k_{yy}, k_{zz}$) and principal moments of inertia ($I_{xx}, I_{yy}, I_{zz}$) of double sphere can be calculated from the following equations:

$$ V = \begin{cases} \frac{4\pi}{3} R^3 (1 - \cos \vartheta^*) & \text{if } \vartheta^* \in [0, 90^\circ] \\ \frac{4\pi}{3} R^3 (1 + \cos \vartheta^*) & \text{if } \vartheta^* \in [90^\circ, 180^\circ] \end{cases} $$

$$ i_{xx} = i_{zz} = 2 \varrho \left\{ \begin{array}{ll} \frac{2\pi}{5} R^5 (1 - \cos \vartheta^*) - \frac{\pi}{5} R^5 \left[ \frac{1}{3} (\cos^3 \vartheta^* - 1) + (1 - \cos \vartheta^*) \right] & \text{if } \vartheta^* \in [0, 90^\circ] \\ \frac{2\pi}{3} (z')^2 R^3 (1 - \cos \vartheta^*) + \frac{\pi}{2} R^4 (z') \sqrt{1 - \cos^2 \vartheta^*} & \text{if } \vartheta^* \in [90^\circ, 180^\circ] \end{array} \right. $$

$$ \varrho R^5 \left[ \frac{2\pi}{3} (z')^2 R^3 (1 + \cos \vartheta^*) + \frac{\pi}{2} R^4 (z') \sqrt{1 - \cos^2 \vartheta^*} \right] $$

$$ i_{yy} = \begin{cases} \frac{4\pi}{5} \varrho R^5 \left[ \frac{1}{3} (\cos^3 \vartheta^* - 1) + (1 - \cos \vartheta^*) \right] & \text{if } \vartheta^* \in [0, 90^\circ] \\ \frac{4\pi}{5} \varrho R^5 \left[ \frac{1}{3} (-\cos^3 \vartheta^* - 1) + (1 + \cos \vartheta^*) \right] & \text{if } \vartheta^* \in [90^\circ, 180^\circ] \end{cases} $$
\[ k_{xx}^2 = k_{zz}^2 = \frac{i_{xx}}{m} = \frac{i_{xx}}{V \varrho} \quad \text{and} \quad k_{yy}^2 = \frac{i_{yy}}{m} = \frac{i_{yy}}{V \varrho} \]

\[ I_{xx} = I_{zz} = mk_{xx}^2 \quad \text{and} \quad I_{yy} = mk_{yy}^2 \]

where:

\( V \) – double sphere’s volume

\( R \) – radius of a single sphere

\( \delta \) – the overlap between two spheres, \( \delta = 2d - md \)

\( z' = R - \frac{\delta}{2} \)

\( \cos \vartheta^* = \frac{z'}{R} \)

\( \varrho \) – particle’s density

\( m \) – particle’s mass

\( y \)-direction was parallel to double sphere’s longitudinal. Two remaining directions (\( x, z \)) were perpendicular to \( y \)-axis and were lying on a plane of symmetry of two spheres, see Fig. 3.32. If we plugged \( \vartheta^* \in [90^\circ, 180^\circ] \) into formulas presented above we would calculate volume, moment of inertia and radii of gyration of double spheres. For \( \vartheta^* \) from the range of \([0, 90^\circ]\) double-spheres start having shape of lenses. Differences between equations describing lenses and double-spheres were marked in red.

Sensitivity analysis of the double-sphere longitudinal dimension impact on the depth at which cone stopped penetrating granular material was conducted on. The outcome of this analysis was shown in Fig. 3.35.
Figure 3.32: Double sphere’s dimensions. $m \in [1.0, \ 2.0]$.

Figure 3.33: Cross-sections of double spheres with different longitudinal dimension. In other words, double spheres having different values of parameter $m$ are presented.

Figure 3.34: Double spheres in isometric view.
Figure 3.35: Depth at which cone stopped penetrating the granular material as a function of double spheres longitudinal dimension. Plot shows results obtained from simulations with cone having $30^\circ$ in its apex angle; cone was dropped from 34.36 mm above the specimen’s surface. inter-particle friction coefficient was set to 0.4 and $\mu_{\text{particle-cone}} = 0.7$. Container’s had a diameter of 6 inches. Dashed lined show depths reached by cones in laboratory tests.
3.3 Standard Triaxial Test

3.3.1 Laboratory Experiments

3.3.1.1 Overview

Detailed description of laboratory standard triaxial test (STT) can be found in [21]. In this section details important from the simulation point of view were presented.

Empirical tests were conducted on using cylindrical container with diameter of 101 mm and height of 203 mm. Two types of granular material were used: first one (monodisperse case) consisted of spheres with 5 mm in diameter; the other one (polydisperse case) was a mixture of evenly distributed spheres with a diameter of 4, 5 and 6 mm. Between 15382 and 15420 beads were used in the laboratory tests.

Particles were made of Grade 25 Chrome Steel of following mechanical parameters: density, \( \rho = 7800 \ \text{kg/m}^3 \); Young’s modulus, \( Y = 2 \cdot 10^{11} \ \text{Pa} \); Poisson ratio, \( \nu = 0.28 \) (Tab. 3.17). Inter-sphere friction coefficient \( (\mu_{\text{particle-particle}}, \mu_{\text{p-p}}) \) as well as coefficient of friction between beads and container’s top and bottom walls \( (\mu_{\text{particle-wall}}, \mu_{\text{p-w}}) \) were measured in [22] and [23], giving values of 0.096 and 0.28, respectively (see Tab. 3.18).

<table>
<thead>
<tr>
<th>Material</th>
<th>( \rho \ [\text{kg/m}^3] )</th>
<th>( Y [\text{Pa}] )</th>
<th>( \nu )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granular material</td>
<td>Grade 25 Chrome Steel</td>
<td>7800</td>
<td>( 2 \cdot 10^{11} )</td>
</tr>
</tbody>
</table>

Table 3.17: Mechanical parameters of particles

<table>
<thead>
<tr>
<th>Contacts' parameters</th>
<th>( \mu_{\text{p-p}} )</th>
<th>( \mu_{\text{p-w}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.096</td>
<td>0.28</td>
</tr>
</tbody>
</table>

Table 3.18: Mechanical parameters describing contacts

Laboratory experiments consisted of two parts. The aim of the first one (settling stage) was to prepare a settled and compressed specimen, which could be used in the second part -
Figure 3.36: Snapshots from simulations of standard triaxial test. Sample after the: (a) settling stage; (b) standard triaxial test stage.

standard triaxial test stage, see Fig. 3.36. Granular material was compressed with confining pressure $p$ of $8 \cdot 10^4$ Pa. When specimen gained its equilibrium state, stress boundary condition on container’s top wall was replaced with an axial strain rate ($\dot{\varepsilon}$) of $0.0083 \%\ s^{-1}$ (Tab. 3.19). Pressure of $8 \cdot 10^4$ Pa on the side walls was kept.

<table>
<thead>
<tr>
<th>$p$ [Pa]</th>
<th>$\dot{\varepsilon}$ [%\ s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lab test parameters</td>
<td>$8 \cdot 10^4$</td>
</tr>
</tbody>
</table>

3.3.1.2 Results

In this section results from empirical tests were summarized. Void ratios of the settled samples were shown in Tab. 3.20. The stress ratio - axial strain curves obtained during the STT tests were presented in Fig. 3.37. Stress ratio is defined as $(\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)$, where:

$\sigma_1$ – axial stress (pressure specimen acts on the top wall with) and

$\sigma_3$ – pressure specimen acts on the side walls with.
Stress ratio is related to the angle of shearing resistance $\phi'$ via following formula:
\[
\sin(\phi') = \frac{(\sigma_1 - \sigma_3)}{(\sigma_1 + \sigma_3)}.
\]
The angle of shearing resistance is e. g. the angle between side and base of the cone formed of a granular material which was poured on the horizontal surface [24].

Table 3.20: Number of spheres used in empirical tests and void ratios of granular material obtained after the settling part

<table>
<thead>
<tr>
<th></th>
<th>Number of Spheres (Void Ratio)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laboratory Experiments</td>
<td>1538 (0.615) ÷ 15420 (0.612)</td>
</tr>
</tbody>
</table>
Figure 3.37: Experimental results. (a) Monodisperse specimen; (b) Polydisperse specimen.
3.3.2 Numerical Simulations

3.3.2.1 Physical Side of the Simulations

Particles were given following mechanical parameters in simulations: density, $\varrho = 7800 \frac{\text{kg}}{\text{m}^3}$; Young’s modulus, $Y = 2 \cdot 10^8 \text{ Pa}$; Poisson ratio, $\nu = 0.28$. Walls of container were treated as massless bodies and their mechanical parameters had the same values as particles (Tab. 3.21).

Table 3.21: Mechanical parameters used in simulations and describing particles and container.

<table>
<thead>
<tr>
<th>Granular material</th>
<th>$\varrho \left[ \frac{\text{kg}}{\text{m}^3} \right]$</th>
<th>$Y \left[ \text{Pa} \right]$</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Container’s walls</td>
<td>massless</td>
<td>$2 \cdot 10^8$</td>
<td>0.28</td>
</tr>
</tbody>
</table>

Friction coefficients between particles and between particles and side walls were set to 0.096. Value of $\mu$ between beads and top and bottom walls was equal to 0.28. Particles were bouncing off of walls and each other with coefficient of restitution of 0.597 [19]. Values of mechanical parameters describing contacts were summarized in Tab. 3.22.

Table 3.22: Mechanical parameters, used in simulations, describing contacts.

<table>
<thead>
<tr>
<th>Contacts’ parameters</th>
<th>$\mu_{p-p}$</th>
<th>$\mu_{p-s}$</th>
<th>$\mu_{p-w}$</th>
<th>$c_{r,p-p}$</th>
<th>$c_{r,p-s}$</th>
<th>$c_{r,p-w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.096</td>
<td>0.096</td>
<td>0.28</td>
<td>0.597</td>
<td>0.597</td>
<td>0.597</td>
</tr>
</tbody>
</table>

Granular material was compressed with an axial strain rate set to $10 \% \text{s}^{-1}$. The reason for giving the axial strain rate value circa 1000 times larger than it was in the empirical tests was to overcome the inconvenience of having long simulation times. To neutralize the effect of compressing the specimen with larger strain rates, grains were treated as softer than they were in reality. Value of beads’ Young’s modulus was set to 1000 times smaller number than the one in Tab. 3.17. Confining pressure of $8 \cdot 10^4 \text{ Pa}$ was used in the numerical calculations.

Similarly to experiments, simulations consisted of two parts: settling stage and standard triaxial test (STT) stage, see Fig. 3.36. In the former one, after pouring the specimen into a container we applied confining pressure, $p = 8 \cdot 10^4 \text{ Pa}$, to its top and side walls. We
Table 3.23: Mechanical parameters describing used in simulation of standard triaxial test.

<table>
<thead>
<tr>
<th></th>
<th>$p$ [Pa]</th>
<th>$\dot{\varepsilon}$ [% s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>STT's parameters</td>
<td>$8 \cdot 10^4$</td>
<td>10</td>
</tr>
</tbody>
</table>

Figure 3.38: Evolution of system’s kinetic energy during the settling stage of standard triaxial test.

Simulation ran until the sample obtained its equilibrium state (Fig. 3.38). Such prepared specimen was used in the latter stage, in which the confining pressure was kept on the side walls and the axial strain rate $\dot{\varepsilon}$ was applied to the top wall. Bottom wall of the container was fixed in both stages.

3.3.2.2 Numerical Side of the Standart Triaxial Test Simulations

General information on numerical side of simulations was given in Section 3.1. In this section we will summarize values of numerical parameters used in simulations of standard triaxial test (Tab. 3.24).
Table 3.24: Values of numerical parameters used in simulations. *MNoI - Maximum Number of Iterations; **CRS - Contact Recovery Speed; ***if calculation in settling stage were done with CRS of 0.02 m/s, then in standard triaxial test stage stability could be obtain for CRS set to larger values (even 10^3 m/s)

<table>
<thead>
<tr>
<th>Approach</th>
<th>Parameter</th>
<th>Monodisperse Sample</th>
<th>Polydisperse Sample</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Settling</td>
<td>STT stage</td>
</tr>
<tr>
<td>DEM-P</td>
<td>$\Delta t [s]$</td>
<td>$3 \cdot 10^{-5}$</td>
<td>$5 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>DEM-C</td>
<td>$\Delta t [s]$</td>
<td>$10^{-4}$</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>MNoI$^*$</td>
<td>700</td>
<td>2500</td>
</tr>
<tr>
<td></td>
<td>CRS$^{**}$ $[m/s]$</td>
<td>$0.02^{**}$</td>
<td>$0.02 \leq$</td>
</tr>
</tbody>
</table>
3.3.2.3 Results

In this section summary of the results from numerical calculations will be presented and compared to the experimental ones. Between 15382 and 15420 spheres were used in laboratory tests, giving void ratios of 0.615 and 0.612, respectively. In simulations to fill out the container we used 15918 spheres in mono- and 15740 in polydisperse case. Void ratios of simulated specimen in its equilibrium state ranged from 0.611 to 0.660, see Tab. 3.25.

Table 3.25: Number of spheres used in numerical calculations. Comparison of void ratios obtained after settling part of simulations and laboratory experiments. Mono. - monodisperse case; Poly. - polydisperse case

<table>
<thead>
<tr>
<th></th>
<th>Spheres</th>
<th>Void Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(Relative Error Range [%])</td>
</tr>
<tr>
<td>Lab. Exp.</td>
<td>15382 ÷ 15420</td>
<td>0.615 ÷ 0.612</td>
</tr>
<tr>
<td>Mono. DEM-P</td>
<td>15918</td>
<td>0.641</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(4.06 ÷ 4.52)</td>
</tr>
<tr>
<td>Mono. DEM-C</td>
<td></td>
<td>0.611</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(0.65 ÷ 0.16)</td>
</tr>
<tr>
<td>Poly. DEM-P</td>
<td>15740</td>
<td>0.660</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(6.82 ÷ 7.27)</td>
</tr>
<tr>
<td>Poly. DEM-C</td>
<td></td>
<td>0.626</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1.76 ÷ 2.24)</td>
</tr>
</tbody>
</table>

A comparison of the experimental and numerical results was illustrated in Fig. 3.39. Data obtained from numerical computation was compared to plots of the variation in stress ratio \((\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)\) as a function of axial strain, published in [25]. The numerical results matched the experimental ones with a fair precision. Additionally, it can be seen that the outcomes from both DEM-P, and DEM-C methods match the experimental ones in final parts of plots (for large axial strains). In the initial part, the discrepancy between DEM-C and experiment can be seen. It can be explained by using a fact that in complementarity approach, particles are modeled as rigid bodies - what makes the specimen stiffer and caused the initial slope of the plot steeper. On the other hand - penalty method captured the physical phenomena of standard triaxial test at every stage of the simulation.
Figure 3.39: Comparison of experimental and numerical results.
3.3.2.4 Performance analysis

Information about the execution time needed to run the standard triaxial test simulations was presented in this sections. As previously said - numerical calculations were divided into two parts - settling and standard triaxial test stage. They took about 0.5 and 1.5 seconds of simulated time, respectively.

Simulations using DEM-P took in average 1 hour 25 minutes for settling stage and 4 hours 55 minutes for standard triaxial test stage (6 hours 20 minutes altogether). Performance of DEM-C-based simulations was following: 9 hours 21 minutes and 44 hours and 14 minutes for settling and STT stage, respectively (53 hours 35 minutes altogether). Simulations were run using 10 threads of Intel i5–4300M CPU @ 2.0 GHz. Results were summarized in Tab. 3.26.

Penalty approach outraced complementarity one when it comes to their performance in simulating standard triaxial test. The reason for having longer execution times when using DEM-C was caused by the large number of iteration (up to 2500) needed to be taken during each time step. Detailed analysis of number of iterations per time step impact on the outcomes was presented in Section 3.3.3.2.

Table 3.26: A comparison of the average execution time of standard triaxial test simulations. LoTS – Length of Time Simulated.

<table>
<thead>
<tr>
<th>Approach</th>
<th>Stage (LoTS [s])</th>
<th>Execution Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>Settling (≈ 0.5)</td>
<td>1 h 25 min</td>
</tr>
<tr>
<td></td>
<td>STT (1.5)</td>
<td>4 h 55 min</td>
</tr>
<tr>
<td></td>
<td>Whole Simulation</td>
<td>6 h 20 min</td>
</tr>
<tr>
<td></td>
<td>(≈ 2.0)</td>
<td></td>
</tr>
<tr>
<td>DEM-C</td>
<td>Settling (≈ 0.5)</td>
<td>9 h 21 min</td>
</tr>
<tr>
<td></td>
<td>STT (1.5)</td>
<td>44 h 14 min</td>
</tr>
<tr>
<td></td>
<td>Whole Simulation</td>
<td>53 h 35 min</td>
</tr>
<tr>
<td></td>
<td>(≈ 2.0)</td>
<td></td>
</tr>
</tbody>
</table>
3.3.3 Additional analyses

3.3.3.1 Impact of the $\mu_{p-s}$ on the results

Simulation of standard triaxial test was sensitive to the value of friction coefficient between container’s side walls and particles ($\mu_{p-s}$). It can be explained that the value of stress ratio (at larger axial strains)

$$f(\sigma_1, \sigma_3) = \frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3}$$

is an increasing function of $\mu_{p-s}$.

In Fig. 3.41 curves obtained for $\mu_{p-s}^1 = 0.096$ lay below ones obtained for $\mu_{p-s}^2 = 0.188$. Values of other mechanical parameters used in those simulations were presented in Tabs. from 3.21 to 3.24. Phenomenon, in which value of stress ratio increases with $\mu_{p-s}$ can be explained from the physical point of view.

First of all, note that $\sigma_3$ does not depend on $\mu_{p-s}$. Value of $\sigma_3$ is dictated by the pressure boundary conditions applied to side walls of container. In simulations conducted on, pressure on side walls was equal to applied confining pressure, $p$. Hence, $\sigma_3 = p = 8 \times 10^4$ Pa in all simulations.

On the other hand, $\sigma_1$ is an increasing function of $\mu_{p-s}$. $\sigma_1$ is a pressure granular material acts in the top wall with. Recall that the sample was compressed with a constant strain rate $\dot{\varepsilon}$. For larger values of $\mu_{p-s}$, granular material kept in a container is less prone to be compressed. Thus, specimen acts on the top wall with larger pressure.

Stress ratio (3.1) is an increasing function of $\sigma_1$, in a domain of our interest: $\sigma_1 \geq \sigma_3$ (see Eq. (3.2) and Fig. 3.40).

$$f(\sigma_1, \sigma_3) = \frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3} = \frac{\sigma_1 + \sigma_3 - 2\sigma_3}{\sigma_1 + \sigma_3} = 1 - \frac{2\sigma_3}{\sigma_1 + \sigma_3}, \sigma_1 \geq \sigma_3 \quad (3.2)$$

Since, stress ratio (3.1) is an increasing function of $\sigma_1$, and $\sigma_1$ is also an increasing function of $\mu_{p-s}$, it implies that stress ratio (3.1) will have larger values for larger $\mu_{p-s}$. Values of $\sigma_1$’s and stress ratios for different $\mu_{p-s}$ were shown in Tab. 3.27. In Fig. 3.40 relation between
Figure 3.40: Stress ratio \((\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)\) as a function of \(\sigma_1\). On the x-axis values of \(\sigma_1\) obtained for \(\mu_{p-s}^1 = 0.096\) and \(\mu_{p-s}^2 = 0.188\), in simulations with polydisperse specimen, were marked; \(\sigma_3 = 80\) kPa.

Table 3.27: Values of \(\sigma_1\) and stress ratio \((\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)\) from the final stage of the standard triaxial test simulation. It can be seen that their values depend on \(\mu_{p-s}\). \(\sigma_3 = 80\) kPa. Mono. - monodisperse, Poly. - polydisperse specimen;

<table>
<thead>
<tr>
<th>(\mu_{p-s})</th>
<th>(\sigma_1) [kPa]</th>
<th>((\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mono.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.096</td>
<td>151</td>
<td>0.307</td>
</tr>
<tr>
<td>0.188</td>
<td>168</td>
<td>0.355</td>
</tr>
<tr>
<td>Poly.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.096</td>
<td>152</td>
<td>0.310</td>
</tr>
<tr>
<td>0.188</td>
<td>176</td>
<td>0.375</td>
</tr>
</tbody>
</table>

stress ratio and \(\sigma_1\) was presented. On x-axis values of \(\sigma_1\) for \(\mu_{p-s}^1 = 0.096\) and \(\mu_{p-s}^2 = 0.188\) were marked. It can be seen that for larger values of \(\mu_{p-s}\), \(\sigma_1\) and \((\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)\) have larger values.
Figure 3.41: Comparison of numerical results for different values of $\mu_{ps}$. 

(a) Monodisperse case.

(b) Polydisperse case.
3.3.3.2 Impact of the MNoI on the results

Settling stage of standard triaxial test simulation using DEM-C approach required at least 700 iterations per time step to make the computations stable and reasonable from the physical point of view. By reasonable we meant having a stable simulation of granular material closed in a container. Additionally sample should act on container’s walls with a pressure equal to confining pressure applied from outside.

Second part of the simulation - standard triaxial stage - required more than 700 iterations per time step to match outcomes obtained from laboratory tests. Numerical calculations with 700 iterations per time step were stable but incorrect from the physical viewpoint, see Fig. 3.42. Simulations with 1000, 1500 iterations (in polydisperse case), and 1000, 1500 and 2000 (in monodisperse one) were unstable. Stability and physical correctness of the results was observed for simulations with MNoI having values larger or equal to 2500 (for monodisperse), and 2000 - for polydisperse specimen (Tab. 3.24 and Fig. 3.42). Outcomes from simulations with MNoI larger than those threshold values were very similar to each other. Sensitivity analysis presented in this section shows that MNoI is a parameter which is not only responsible for stability of calculations, but it is also important when it comes to modeling the mechanical systems from the physical viewpoint.
Figure 3.42: Comparison of numerical results from simulations with different number of iterations per time step.
3.4 Direct Shear Test with Particle Image Velocimetry

3.4.1 Laboratory Experiments

3.4.1.1 Overview

Detailed report concerning laboratory direct shear test can be found in [26]. In this section aspects of the test which needed to be considered during the numerical modeling were described. Mechanical parameters and geometrical dimensions of bodies used in empirical tests were also provided.

Experiments were conducted on using a shear box divided horizontally. To allow for tracking of individual grains (i) granular material consisted of only one layer of particles and (ii) shear box was given a transparent front wall to enable capturing the motion of glass beads with a digital camera.

The container consisted of the following parts made of Plexiglas:

1. shear box, consisting of one fixed (bottom) and one moving (top) frame,

2. transparent front wall (mentioned above),

3. top plate, which was exerting a normal force on the top of sheared granular material,

4. plate (or base) which could be inclined at certain angles; shear box was placed on this plate.

Shear box was 101.96-mm-wide; its fixed half was 50.58-mm-deep and the distance between front wall and base plate was 3.3 mm. Top plate had following dimensions: $100 \times 25 \times 3.25$ mm (Tab. 3.28).

Shear box was filled out with a dry granular material made of imperfect spheres. Those imperfect spheres were made of glass and could be modeled as ellipsoids of diameters from the following normal distribution: $N(2.84, 0.0834)$ mm (Tab. 3.29).
Table 3.28: Dimensions of container and top plates used in laboratory tests.

<table>
<thead>
<tr>
<th>Container’s Parts</th>
<th>Top Frame</th>
<th>Bottom Frame</th>
<th>Top Plate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width [mm]</td>
<td>101.96</td>
<td>101.96</td>
<td>100.00</td>
</tr>
<tr>
<td>Depth/Length [mm]</td>
<td>–</td>
<td>50.58</td>
<td>25.00</td>
</tr>
<tr>
<td>Gap Size/Thickness [mm]</td>
<td>3.30</td>
<td>3.30</td>
<td>3.25</td>
</tr>
</tbody>
</table>

Granular material in two different compactions – loose and dense – was used in the experiments. In dense case, between 1303 and 1310 grains were arranged in one layer via hexagonally close packing. In loose case, shear box was filled out with 1174 to 1214 particles under arbitrary packing, see Fig. 3.43.

Normal force was applied to the shear plane by inclining the apparatus and adding a mass on top of the granular material – via placing a top plate on it. Shear box was inclined at three different angles (18°, 24°, 30°); top plates of 8.01 g, 53.64 g, 66.64 g were used. The top frame was given two shearing speeds: 0.5 mm/min and 1.0 mm/min. For each packing compaction a set of six tests, summarized below, was run. The apparatus was inclined at:

- 18° with no top plate placed on the granular material for both shear rates,
- 24° with 8.01 g of additional mass for both shear rates and
- 30° with top plate of
  - 66.64 g for 0.5 mm/min shearing speed and
  - 53.64 g for 1.0 mm/min shearing speed

In every test, trajectories of six chosen particles were monitored. Their horizontal and vertical position were calculated with respect to one of the five markers located on the ground plate (the bottom left one; see Fig. 3.43).
Figure 3.43: Snapshots from laboratory test. Particles packed: (a) densely; (b) loosely.

Table 3.29: Dimensions and material of particles used in laboratory tests.

<table>
<thead>
<tr>
<th>Granular material</th>
<th>Shape</th>
<th>Diameters distribution [mm]</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ellipsoids</td>
<td>N(2.84, 0.0834)</td>
<td>Glass</td>
<td></td>
</tr>
</tbody>
</table>

3.4.1.2 Results

Experimental results, published in [26], were presented in this section.
Figure 3.44: Trajectories of selected particles obtained from laboratory experiments. Two plots are provided in each sub-figure; left and right plots are obtained for $V_{sh} = 0.5$ mm/min and $V_{sh} = 1.0$ mm/min, respectively. Particles packed **densely** and shear box inclined at: (a) 18°; (b) 24°; (c) 30°.
Figure 3.45: Trajectories of selected particles obtained from laboratory experiments. Two plots are provided in each sub-figure; left and right plots are obtained for $V_{sh} = 0.5$ mm/min and $V_{sh} = 1.0$ mm/min, respectively. Particles packed loosely and shear box inclined at: (a) 18°; (b) 24°; (c) 30°.
3.4.2 Numerical Simulations

3.4.2.1 Physical Side of the Simulations

Simulations of direct shear test were divided into two parts. The aim of the first one, called settling stage, was having a container filled out with a granular material in its equilibrium state. To obtain such samples, of two different packings (loose and dense), two different source codes were used.

Dense compaction was achieved by arranging particles in one-layer-grid via hexagonally close packing (34 or 35 elements per each of 38 rows, giving 1311 elements in whole grid). Such granular material was placed in a container inclined at a certain angle. Due to the fact that container’s width was larger than the width of the grid (in both laboratory and numerical tests), the arrangement of settled particles was not exact but very similar to the hexagonal close one.

To obtain loose compaction, granular material (1154 particles) was poured into the container and was allowed to gain its equilibrium state. Since the top surface of the sample was not flat, a couple of granular material’s top rows were removed from the simulation making its surface flat. Then, the top plate was placed on the granular material and the sample was allowed to gain its equilibrium one more time.

Specimens, prepared in the way described above, were used in the second part of the simulation, called direct shear stage. During this stage, the top frame of the box was moving with one of two considered speeds (0.5 or 1.0 mm/min), causing shearing of the granular material. Similarly to laboratory tests, trajectories of 6 particles were monitored in every simulations. Those 6 particles were chosen based on the distances of their initial positions and the initial positions of particles monitored during the empirical experiments. The particles corresponding to the shortest distances were chosen.

Shear box used in the numerical simulations was massless and had the same geometrical dimensions as the one used in laboratory experiments. Masses and geometrical dimensions of top plates were the same as those from the laboratory tests.
Granular material consisted of perfect spheres with diameters of 2.84 mm. Particles were made of glass having following mechanical parameters: density, $\rho = 2500 \frac{\text{kg}}{\text{m}^3}$; Young’s modulus $Y = 50 \times 10^9 \text{ Pa}$; Poisson’s Ratio $\nu = 0.3$. Mechanical parameters of container’s walls were given the same values. Coefficients of restitution between particles and between particles and walls were set to 0.658 [19]. Corresponding friction coefficients were equal to 0.7 [20], see Tabs. 3.30 and 3.31.

Table 3.30: Mechanical parameters of particles used in simulations.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\rho \left[ \frac{\text{kg}}{\text{m}^3} \right]$</th>
<th>$Y \left[ \text{Pa} \right]$</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Granular material</td>
<td>Glass</td>
<td>2500</td>
<td>$50 \times 10^9$</td>
</tr>
</tbody>
</table>

Table 3.31: Mechanical parameters describing contacts used in simulations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\mu_{p-p}$</th>
<th>$\mu_{p-w}$</th>
<th>$c_{r,p-p}$</th>
<th>$c_{r,p-w}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.7</td>
<td>0.7</td>
<td>0.658</td>
<td>0.658</td>
</tr>
</tbody>
</table>

3.4.2.2 Numerical Side of the Direct Shear Test Simulations

General information on numerical side of simulations was given in Section 3.1. In this section values of the numerical parameters used in simulations of direct shear test were presented, see Tab. 3.32.

Table 3.32: Values of numerical parameters used in simulations. *MNoI - Maximum Number of Iterations; ** CRS - Contact Recovery Speed.

<table>
<thead>
<tr>
<th>Case</th>
<th>Approach</th>
<th>time step [s]</th>
<th>MNoI*</th>
<th>CRS** [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dense</td>
<td>DEM-P</td>
<td>$2 \times 10^{-6}$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>DEM-C</td>
<td>$9 \times 10^{-4}$</td>
<td>500</td>
<td>1.0</td>
</tr>
<tr>
<td>Loose</td>
<td>DEM-P</td>
<td>$2 \times 10^{-6}$</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>DEM-C</td>
<td>$2 \times 10^{-4}$</td>
<td>200</td>
<td>1.0</td>
</tr>
</tbody>
</table>
After a closer analysis of Tab. 3.32, reader could ask a question why different values of maximum number of iterations were used in simulations with granular material packed loosely (MNoI = 200) and densely (MNoI = 500). The answer is following: in dense case, particles were arranged in a controlled way (via hexagonal closed packing). This is a reason why their motion could be determined a priori, and more iterations per time step were needed in providing results correct from physical view point (or matching experimental data).

On the other hand, granular material packed loosely introduces certain randomness to the mechanical system. This randomness is caused by a lack of control on the initial arrangement of settled particles, which were poured into the container. Thus, even though less iterations per time step were taken, results matched experimental data to a satisfactory extent. In other words, the randomness present in mechanical system allowed us to take less number of iterations per time step and still keep the results in an acceptable range of correctness.
3.4.2.3 Results

In this section results obtained from simulations of direct shear test with PIV were presented and compared to the experimental data published in [26]. During the experiments and simulations trajectories of six particles were monitored, see Figs. 3.47 and 3.48.

When it comes to the empirical tests with granular material packed loosely, experimental data comes from single experiments (i.e. one test for each of six cases: 3 inclined angles \times 2 shearing speeds). Based on the results coming from simulations, we observed that the initial arrangement of particles can impact the trajectories. Even if two samples are considered as packed loosely, different initial arrangements of their particles can impact sample’s anisotropy. This implies shearing planes of different orientations occurring in different places. We believe that running more than one experiment for each of six above-mentioned cases and calculating an average trajectories would be useful.

We decided to run four different scenarios of shear test with loosely packed fill-out; in each scenario initial arrangement of particles was random. Numerical results presented in this section are average results of those four scenarios, see Fig. 3.48. Outcomes coming from four above-mentioned scenarios were presented in Section 3.4.3.2.

Similarly to the experiments with granular material packed loosely, the results from dense case scenario come from single experiments (i.e. one test for each of six cases: 3 inclined angles \times 2 shearing speeds). Since, there was no factor of randomness in the initial arrangement of particles (they always formed a hexagonally-close-packed grid), one run of empirical (as well as numerical) test was enough.

Shearing speeds used in the laboratory tests were low (0.5 and 1.0 mm/min) and led to lengthy experiments, which needed to be duplicated in simulations. A pilot simulations using complementarity and penalty approaches were carried out at the actual lab shearing speeds. They took about 23 days to complete using DEM-C and would take approximately 54 days using DEM-P. This is a reason why the sensitivity analysis with respect to the shearing speed \( V_{sh} \) was conducted on. The purpose of the analysis was to understand to what extent
(a) Granular material packed loosely; incline angle of $18^\circ$; shearing speed of 1.0 mm/min.

(b) Granular material packed densely; incline angle of $24^\circ$; shearing speed of 0.5 mm/min.

Figure 3.46: Particle arrangement comparison at the end of the shear test. Snapshots come from: experiment (top); simulation (bottom); random loose packing (left); hexagonal closed packing (right). Trajectories of six particles, marked in red, were monitored.
increase of the shearing speed would impact the numerical results. All simulations were run using one thread on an i5-4300M CPU @ 2.0 GHz processor.

Results from simulations based on both DEM-P and DEM-C showed little sensitivity to shearing velocity. We managed running DEM-P-based simulations for $V_{sh,sim} \geq 4$ mm/min; i.e., shearing speed at least four times faster than the experimental one. Since DEM-C-based simulations were from two to six times faster than those using DEM-P (see Tabs. 3.33 and 3.34), we managed to run some of them with $V_{sh}$ equal to the actual speed used in laboratory, $V_{sh,sim} = V_{sh,exp}$. Different shearing speeds did not lead to big changes in particles trajectories (maybe except for simulations with a sample packed densely in shear box inclined at 18°). We also observed that the numerical results coming from DEM-C-based simulations were closer to the experimental ones when $V_{sh,sim}$ was faster.

In Figs. 3.47 and 3.48 numerical results were presented and compared to the experimental data. Outcomes coming from simulations where shearing velocity was 500 times larger than the one used in lab tests were presented. Additionally, we showed trajectories coming from simulations with the slowest $V_{sh,sim}$’s we managed to run the simulations with, and keep the execution time reasonable. DEM-C was fast enough to allow us running simulations with the actual lab shearing speed (it took at most 23 days; thus $\alpha = \beta = 1$). Simulations using DEM-P were slower (54 days at most) so we run simulations of dense case with $V_{sh,sim} \geq 8$ mm/sec ($\alpha = 16$, $\beta = 8$) and with $V_{sh,sim} \geq 4$ mm/sec of loose case ($\alpha = 8$, $\beta = 4$). Results for $V_{sh,sim} \times 500$ were presented to show that they match experimental data better when DEM-C is used, and that DEM-P-based simulations are not very sensitive to values of $V_{sh,sim}$. 
Figure 3.47: Trajectories of selected particles obtained from simulation and lab experiments. Particles packed densely. Shear box inclined at: (a) 18° (b) 24° (c) 30°. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.

Two sets of trajectories obtained in simulations were presented. First set presents the results with shearing velocity 500 times larger than the one used in laboratory ($V_{sh} \times 500$). Second set consists of results obtained for the simulations with shearing velocities closer to those used in experiments. Due to the long execution times of simulations based on DEM-P, the slowest shearing velocities were equal to 8 mm/min (i.e. $V_{sh,\text{sim}} \geq 8$ mm/min; $\alpha = 16$, $\beta = 8$). Computations using DEM-C were faster and allowed sample to be sheared with velocities used in empirical test ($\alpha = \beta = 1$).
Figure 3.48: Trajectories of selected particles obtained from simulation and lab experiments. Particles packed loosely. Shear box inclined at: (a) 18° (b) 24° (c) 30°. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min. Two sets of trajectories obtained in simulations were presented. First set presents the results with shearing velocity 500 times larger than the one used in laboratory ($V_{sh} \times 500$). Second set consists of results obtained for the simulations with shearing velocities closer to those used in experiments. Due to the long execution times of simulations based on DEM-P, the slowest shearing velocities were equal to 4 mm/min (i.e. $V_{sh,sim} \geq 4$ mm/min; $\alpha = 8, \beta = 4$). Computations using DEM-C were faster and allowed sample to be sheared with velocities used in empirical test ($\alpha = \beta = 1$).
3.4.2.4 Performance analysis

Execution time of direct shear test with PIV simulation is discussed in this section. As mentioned previously, simulations consisted of two parts: settling and direct shear stages. Two different source codes were used in simulating settling part with granular material packed densely and loosely. The latter stage was identical for both cases.

In settling stage with granular material packed densely, particles were arranged in single-layered grid via hexagonally packing. They were placed in a shear box with a plate on their surface (this top plate was present only in simulations with apparatus inclined at 24° and 30°). Sample prepared in such way were given 1.0 second of simulation time to gain their equilibrium state.

In the loose case, granular material was poured into the container and was given 1 second of time simulated to gain its equilibrium. Free surface of the settled sample was not flat, thus a couple of granular material’s top rows were removed from simulation. After making the top surface flat, top plate was placed on the sample’s surface and mechanical system was allowed to gain its equilibrium state once again (1 second of simulation time).

Such samples of settled granular material were used in the second part of simulation, called direct shear test stage. As written in Section 3.4.2.3, sensitivity analysis of shearing velocity impact on the results was conducted on. The reason we mentioned about it in a section about performance is that the simulations with slower shearing velocities took more simulation time (what naturally impacted execution time as well).

For example, numerical calculations with the actual shearing velocity \(V_{sh,sim} = 1.0\ mm/min\) last 600 seconds (10 minutes) of simulation time. Simulation with 500 times faster sharing velocity \(V_{sh,sim} = 1.0 \times 500\ mm/min\) last 1.2 seconds only. Simulations with \(V_{sh,sim} = 0.5 \times \alpha\ mm/min\) (where \(\alpha \in \{1, \ldots, 500\}\)) were twice longer than the corresponding simulations with \(V_{sh,1.0}\). E. g., they took 2.4 seconds of simulation time when \(V_{sh,sim} = 0.5 \times 500\ mm/min\) or 1200 seconds (20 minutes) when \(V_{sh,sim} = 0.5\ mm/min\).
The analysis of performance showed that simulations based on DEM-C were from 2 to 6 times faster than ones based on DEM-P. All simulations were run using 1 thread of an Intel ES-2650 v3 @ 2.30 Ghz. Results were summarized in Tabs. from 3.33 to 3.34.

Table 3.33: A comparison of execution time of computations using penalty and complementarity approaches. Particles packed densely. Simulations with 1311 bodies. Length of execution times for calculations with \( V_{sh0.5} \) would be twice longer.

<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Length of Time Simulated (LoTS) [s]</th>
<th>Execution time</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>1.0</td>
<td>1 h 9 min</td>
</tr>
<tr>
<td>DEM-C</td>
<td>13 min</td>
<td></td>
</tr>
</tbody>
</table>

Direct Shear Stage

<table>
<thead>
<tr>
<th>Shearing Velocity</th>
<th>Length of Time Simulated (LoTS)</th>
<th>Execution time</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{sh1.0} \times 500 ) ( V_{sh1.0} )</td>
<td>1.2 seconds 600 seconds (10 min)</td>
<td>1 h 21 min ≈ 27 days</td>
</tr>
<tr>
<td>( V_{sh1.0} \times 500 ) ( V_{sh1.0} )</td>
<td>1.2 seconds 600 seconds (10 min)</td>
<td>22 min 4 days 18 hours</td>
</tr>
</tbody>
</table>

Table 3.34: A comparison of execution time of computations using penalty and complementarity approaches. Particles packed loosely. Simulations with 1154 bodies. Length of execution times for calculations with \( V_{sh0.5} \) would be twice longer.

<table>
<thead>
<tr>
<th>Settling Stage</th>
<th>Length of Time Simulated (LoTS) [s]</th>
<th>Execution time</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM-P</td>
<td>1.0</td>
<td>43 min</td>
</tr>
<tr>
<td>DEM-C</td>
<td>1.0</td>
<td>58 min</td>
</tr>
<tr>
<td>Whole Simulation</td>
<td>2.0</td>
<td>1 h 41 min</td>
</tr>
</tbody>
</table>

Direct Shear Stage

<table>
<thead>
<tr>
<th>Shearing Velocity</th>
<th>Length of Time Simulated (LoTS)</th>
<th>Execution time</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{sh1.0} \times 500 ) ( V_{sh1.0} )</td>
<td>1.2 seconds 600 seconds (10 min)</td>
<td>1 h 4 min ≈ 25 days</td>
</tr>
<tr>
<td>( V_{sh1.0} \times 500 ) ( V_{sh1.0} )</td>
<td>1.2 seconds 600 seconds (10 min)</td>
<td>34 min 11 days 16 hours</td>
</tr>
</tbody>
</table>
3.4.3 Additional Analyses

3.4.3.1 Impact of the initial arrangements of particles on the results

In this section we presented results coming from simulations of four scenarios of direct shear test with granular material packed loosely. Each of those scenarios differs from each other in initial arrangement of particles. In Figs. 3.49 - 3.52 we showed four sets of plots, each set corresponds to one of those initial arrangements. Those plots showed that different initial positions of grains impacts trajectories of six monitored particles.

Additionally, in every plot results concerning sensitivity analysis of shearing velocity were showed. Shearing speeds used in the laboratory tests were low (0.5 and 1.0 mm/min) and led to lengthy experiments, which needed to be duplicated in simulations. A pilot simulations using complementarity and penalty approaches were carried out at the actual lab shearing speeds. They took about 23 days to complete using DEM-C and would take approximately 50 days using DEM-P (Tab. 3.34). This is a reason why the sensitivity analysis with respect to the shearing speed $V_{sh}$ was conducted on. The purpose of the analysis was to understand to what extent increase of the shearing speed would impact the numerical results.

Results from simulations based on both DEM-P and DEM-C showed little sensitivity to shearing velocity. We managed running DEM-P-based simulations for $V_{sh,sim} \geq 4$ mm/min; i.e., shearing speed at least four times faster than the experimental one. Since DEM-C-based simulations were about two times faster than those using DEM-P (see Tab.3.34), we managed to run some of them with $V_{sh}$ equal to the actual speed used in laboratory, $V_{sh,sim} = V_{sh,exp}$. Different shearing speeds did not lead to big changes in particles trajectories.
Figure 3.49: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed loosely and with initial arrangement of its particles from Scenario 1. Shear box inclined at: (a, b) $18^\circ$; (c, d) $24^\circ$; (e, f) $30^\circ$. Simulations using: (a, c, e) DEM-P and (b, d, f) DEM-C approaches. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.
Figure 3.50: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed loosely and with initial arrangement of its particles from Scenario 2. Shear box inclined at: (a, b) 18°; (c, d) 24°; (e, f) 30°. Simulations using: (a, c, e) DEM-P and (b, d, f) DEM-C approaches. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5 \text{ mm/min}$ and right one $V_{sh} = 1.0 \text{ mm/min}$. 
Figure 3.51: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed loosely and with initial arrangement of its particles from Scenario 3. Shear box inclined at: (a, b) 18°; (c, d) 24°; (e, f) 30°. Simulations using: (a, c, e) DEM-P and (b, d, f) DEM-C approaches. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.
Figure 3.52: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed loosely and with initial arrangement of its particles from Scenario 4. Shear box inclined at: (a, b) 18°; (c, d) 24°; (e, f) 30°. Simulations using: (a, c, e) DEM-P and (b, d, f) DEM-C approaches. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.
3.4.3.2 Impact of the shearing velocity on the results of dense case

In this section results concerning sensitivity analysis of shearing velocity were described. The results came from simulations of direct shear test with granular material packed densely. In opposite to numerical tests with granular material packed loosely – there was no need for running multiple simulations and calculations average trajectories of monitored particles. Here, granular sample was arranged in one layer via hexagonally close packing. Because of such arrangement of initial positions, motion of particles was determined a priori. Thus, to find trajectory of certain particle it was enough to run only one simulation.

Shearing speeds used in the laboratory tests were low (0.5 and 1.0 mm/min) and led to lengthy experiments, which needed to be duplicated in simulations. A pilot simulations using complementarity and penalty approaches were carried out at the actual lab shearing speeds. They took about 10 days to complete using DEM-C and would take approximately 54 days using DEM-P (see Tab. 3.33). This is a reason why the sensitivity analysis with respect to the shearing speed $V_{sh}$ was conducted on. The purpose of the analysis was to understand to what extent increase of the shearing speed would impact the numerical results.

Results from simulations based on both DEM-P and DEM-C showed little sensitivity to shearing velocity. We managed running DEM-P-based simulations for $V_{sh,sim} \geq 8$ mm/min; i.e., shearing speed at least eight times faster than the experimental one. Since DEM-C-based simulations were about six times faster than those using DEM-P (see Tabs. 3.33), we managed to run them with $V_{sh}$ equal to the actual speed used in laboratory, $V_{sh,sim} = V_{sh,exp}$. Different shearing speeds did not lead to big changes in particles trajectories (maybe except for simulations with a sample in shear box inclined at 18°). We also observed that the numerical results coming from DEM-C-based simulations were closer to the experimental ones when $V_{sh,sim}$ was faster.
Figure 3.53: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed densely. Simulations based on DEM-P method. Shear box inclined at: (a,) $18^\circ$; (b) $24^\circ$; (c) $30^\circ$. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.
Figure 3.54: Sensitivity analysis of shearing velocity impact on the trajectories of monitored particles. Granular material packed densely. Simulations based on DEM-C method. Shear box inclined at: (a) $18^\circ$; (b) $24^\circ$; (c) $30^\circ$. Two plots are provided in each sub-figure; left plot corresponds to $V_{sh} = 0.5$ mm/min and right one $V_{sh} = 1.0$ mm/min.
4 CONCLUSION AND FUTURE WORK

Based on the results from simulations of cone penetration, standard triaxial and direct shear tests, it can be said that both DEM-P and DEM-C approaches can be used in simulations of geomechanical tests. If calibrated correctly, penalty and complementarity approaches can give results which are close to the experimental ones and to one another.

When it comes to the performance of those two methods, DEM-P-based algorithms were faster than DEM-C-based ones in simulations of cone penetration ($\approx 2\times$) and standard triaxial ($\approx 10\times$ faster) tests. Shorter execution times were mainly caused by the possibility of taking larger time steps in simulations using penalty approach, what implied a speedup of computations. Taking larger $\Delta t$'s was possible thanks to the relaxation of grains stiffness (Young’s modulus about 1000 times smaller than in reality). On the other hand, in computations concerning direct shear test particles were given real elastic moduli values (i. e. Young’s modulus of glass particles $\propto 10^{10}$ Pa). Simulations of granular material with Young’s modulus value of this order required very small time steps ($\Delta t \propto 10^{-6}$ sec.). It resulted in having long execution times of computations using penalty approach. Thus, simulations of direct shear test based on DEM-C were even up to 6 times faster than those based on DEM-P. We believe that the performance of complementarity based simulations can be improved, mainly by making the algorithm, used in solving the optimization part of the model, more effective.

Besides simulating actual laboratory tests, we analyzed the impact of certain numerical and mechanical parameters on the results. We observed that the coefficient of friction between particles has noticeable impact on the density of settled material’s packing. Additionally, it influenced motion of the cone dropped onto a granular material (cone stopped penetrating the sample earlier when $\mu_{p-p}$ was larger). Surprisingly, friction coefficient between particles and cone had very little impact on the results.

In standard triaxial test, results were sensitive to the coefficient of friction between particles and side walls. Additionally, we noticed that the number of iterations done in every
time step (in simulations using complementarity approach) impacted not only the stability of calculations, but also the correctness of results from physical point of view.

When it comes to the simulations of direct shear test with PIV, an analysis of shearing velocity impact on the results was carried out. It turned out that most of the calculations were little sensitive to this parameter. Results from simulations using DEM-C approach were, surprisingly, closer to the experimental ones when $V_{sh}$ was faster than the one used during the lab tests. We also noticed that the trajectories of monitored beads depended on the initial configuration of particles of settled granular material.

Work presented in this thesis showed that the penalty and complementarity based discrete element methods can be successfully used in simulations of geomechanical tests. This outcome is quite remarkable, since both of those methods handle friction and contact using vastly different ways, either from physical or numerical angles.
5 NOMENCLATURE

Abbreviations

DEM-P  Discrete Element Method - Penalty
DEM-C  Discrete Element Method - Complementarity
CPT    Cone Penetration Test
STT    Standard Triaxial Test
DST    Direct Shear Test
PIV    Particle Image Velocimetry

Notation

\( a \) Scalar
\( \mathbf{a} \) Vector
\( A \) Matrix
\( A_{m \times n} \) Matrix \( A \) of Size \( m \times n \)
\( A^T \) Transpose of Matrix \( A \)
\( |a| \) Magnitude of Vector \( a \)
\( \mathbf{a} \) Vector \( a \) Expressed in Local Frame
\( \tilde{a} \) Skew-Symmetric Matrix Generated from Vector \( a \)
\( \dot{a} \) Total Time Derivative of Vector \( a \)
\( \mathbf{a}_t \) Partial Time Derivative of Vector \( a \)
\( \mathbf{a}_q \) Partial Derivative of Vector \( a \) w. r. t. vector \( q \) (Jacobi Matrix)
\( a \circ b \) Scalar Product of \( a \) and \( b \)
\( a \times b \) Cross Product of \( a \) and \( b \)
\( a^{(l)} \) Vector \( a \) Evaluated in \((l)\)-th Time Step

Parameters Describing DEM-P

\( \mathbf{F} \) Contact Force
\( F_n \) Normal Component of \( \mathbf{F} \)
\( F_t \) Tangential Component of \( \mathbf{F} \)
\( F_n \) Magnitude of \( F_n \)
\( F_t \) Magnitude of \( F_t \)
\( \mathbf{n} \) Unit Normal Vector at Contact
t Unit Tangential Vector at Contact
$k_n$ Normal Stiffness Coefficient
$k_t$ Tangential Stiffness Coefficient
$\gamma_n$ Normal Damping Coefficient
$\gamma_t$ Tangential Damping Coefficient
$\delta_n$ Overlap/Gap Size/Penetration Gap
$\delta_t$ Tangential Contact Displacement
$\delta_t^m$, $\delta_t$ in Current Time Step
$\gamma_n$ Normal Damping Coefficient
$\gamma_t$ Tangential Damping Coefficient
$v_{rel}$ Relative Velocity
$v_{rel,n}$ Normal Component of $v_{rel}$
$v_{rel,t}$ Tangential Component of $v_{rel}$
v_{rel,n} Magnitude of $v_{rel,n}$
v_{rel,t} Magnitude of $v_{rel,t}$
$\omega_i$ Angular Velocity of Body $i$
s_i Vector Pointing From Contact Point to Center of Mass of $i$-th Body
$\Delta t$ Time Step
$m_{eff}$ Effective Mass
$R_{eff}$ Effective Radius
$Y_{eff}$ Effective Young’s Modulus
$G_{eff}$ Effective Shear Modulus
$c_r$ Coefficient of Restitution
$m_i$ Mass of $i$-th Body
$R_i$ Radius of Curvature at Contact Point of $i$-th Body
$Y_i$ Young’s Modulus of $i$-th Body
$\nu_i$ Poisson’s Ratio of $i$-th Body
$\mu$ Coefficient of Friction

**Parameters Describing DEM-C**

$n_b$ Number of Bodies
$n_c$ Number of Contacts
$n_{bi}$ Number of Bilateral Constraints
$q$ Vector of Generalized Coordinates with Orientations Expressed by Euler Parameters
$v$ Vector of Generalized Velocities with Angular Velocities Expressed in Local Frame
L Mapping from $v$ to $q$

B Mapping from $\dot{\epsilon}$ to $\omega$
$\epsilon$ Euler Parameters
$\omega$ Angular Velocity
$I$ Identity Matrix
$M$ Mass Matrix
$m_i$ Mass of $i$-th Body
$J_i$ Moment of Inertia Matrix of $i$-th Body
F Applied Forces and Torques
Vector of Lagrange Multipliers Associated with Bilateral Constraints

Vector of Lagrange Multipliers Associated with Unilateral Constraints

Contact Space Generator Matrix

Rotation Matrix

Vector Pointing From $k$-th Contact Point to Center of Mass of $i$-th Body

Gap Function at $i$-th Contact

Magnitude of Normal Force at $i$-th Contact

Vector of Tangential Force at $i$-th Contact

Vector of Relative Tangential Velocity at $i$-th Contact

Coefficient of Friction at $i$-th Contact

time step

Parameters Shared by All Simulations

Physical Parameters

density

Young’s modulus

Poisson’s ratio

inter-particle friction coefficient

friction coefficient between and particles and walls of container

inter-particle coefficient of restitution

coefficient of restitution between and particles and walls of container

Numerical Parameters

time step

MNoI Maximum Number of Iterations

Contact Recover Speed

Parameters Used in Cone Penetration Test Simulations

friction coefficient between particles and cones

coefficient of restitution between particles and cones
\[ L_i \text{ cones' altitude; } i \in \{30^\circ, 60^\circ\} \]
\[ W_i \text{ diameter of cones' base; } i \in \{30^\circ, 60^\circ\} \]
\[ H \text{ initial height cones were dropped from } \]
\[ (H \in \{0, \frac{1}{2} L_i, L_i\}, i \in \{30^\circ, 60^\circ\}) \]
\[ g \text{ Earth's gravity} \]

**Parameters Used in Standard Triaxial Test Simulations**

- \( p \) confining pressure
- \( \dot{\varepsilon} \) axial strain rate
- \( \sigma_1 \) axial stress
- \( \sigma_3 \) pressure specimen acts on containers side walls with
  \[ \phi' \] angle of shearing resistance;
  \[ \sin(\phi') = (\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3) \]
- \( \mu_{p-w} \) coefficient of friction between particles and container’s side walls
- \( \mu_{p-w} \) coefficient of restitution between particles and container’s top and bottom walls
- \( \mu_{p-w} \) coefficient of friction between particles and container’s top and bottom walls

**Parameters Used in Direct Shear Test Simulations**

- \( V_{sh} \) shearing velocity
- \( V_{sh,0.5} \) shearing velocity of 0.5 mm/min used in simulations
- \( V_{sh,1.0} \) shearing velocity of 1.0 mm/min used in simulations
- \( V_{sh,exp} \) shearing velocity used in experiments;
  \[ V_{sh,exp} \in \{0.5, 1.0\} \text{ mm/min} \]
BIBLIOGRAPHY


