A Coupled DEM-LBM approach to simulate saturated sands

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ABSTRACT. *We present a 3D model to analyse the micromechanical behavior of saturated granular materials under dynamic conditions. Among the possible applications of this model include the study of sands in quick and liquefaction conditions. The solid grains assumed spherical, are modeled using Discret Element Method (DEM). Saturating fluid flow and the hydrodynamic forces generated on the grains are modeled using the Lattice Boltzmann Method (LBM). Specific aspects to the coupling of the two methods for taking into account the interaction of the two phases are developed. The numerical applications performed show satisfactory results.*

RÉSUMÉ. *Dans ce travail, on présente un modèle 3D pour l'analyse micromécanique de la réponse des milieux granulaires saturés, soumis à des sollicitations dynamiques. Parmi les applications possibles de ce modèle, on peut citer l'étude des phénoménes de boulance et de liquéfaction des sables. Les grains solides, supposés de forme sphérique sont modélisés en utilisant la Méthode des Eléments Discrets (DEM). Les écoulements du fluide saturant ainsi que les forces hydrodynamiques engendrées sur les grains sont modélisés en utilisant la Méthode Lattice Boltzmann (LBM). Des aspects spécifiques au couplage des deux méthodes pour la prise en compte de l'interaction des deux phases sont développés. Les applications numériques réalisées montrent des resultats satisfaisants.*

KEYWORDS: *saturated granular media, dynamic behavior, discret elements, lattice Boltzmann.*

MOTS-CLÉS : *milieux granulaires saturés, comportement dynamique, éléments discrets, lattice Boltzmann.*

1. Introduction

Discrete Element modeling of granular materials containing a liquid phase has received a great interest in recent years. In the case of non-saturated (wet) materials, the DEM is usually applied by adding capilar forces to model the liquid phase effects (Richefeu *et al.*, 2006). For saturated materials, fluid flows that are induced by the particles displacements has crucial effects on the material's behavior. Therefore a convenient fluid modeling is required in addition to discret element modeling of grains. In the last two decades, the LBM has emerged as a powerful tool to model fluid flows in complex geometries. This method has been coupled in different ways with DEM in order to simulate saturated granular materials behavior (Feng *et al.*, 2007). In this paper we present a 3D coupled DEM-LBM model to simulate saturated granulars and suspended particles. Solid particules are modeled as discrete elements. Saturating fluid flow is modeled using the LBM, the fluid-grains interaction; i.e. the fluid flow boundary conditions and the hydrodynamic forces on grains, is taken into account by imposing a no slip condition between the two phases (fluid and grains). This condition is imposed through the "Interpolated Bounce Back" IBB rule proposed by Bouzidi et al. (Bouzidi *et al.*, 2001).

In the following we describe the model in three sections, the first section describes the DEM briefly, the second presents the LBM, with the curved moving boundary treatment used to model fluid-solid interaction and the third section gives the important issues of the DEM and LBM coupling. The paper ends with a presentation of some results and validations of the model.

2. Discret element modeling of interaction between moving particles

In this work, we use the Smooth Discrete Element Method (SDEM) (Cundall *et al.*, 1979). This method is based on the concept that individual material elements are considered to be separate and interact with each other only along their boundaries by appropriate physically based interaction laws. Thus a particle's motion can be described through Newton's equations

$$m\mathbf{a} = \mathbf{F}_c + \mathbf{F}_{ext} + m\mathbf{g}, \qquad \mathbf{J}\dot{\omega} = \mathbf{M}_c + \mathbf{M}_{ext} \qquad [1]$$

where m and $\mathbf{J}$ are respectively the particle's mass and moment of inertia matrix, $\mathbf{a}$ and $\dot{\omega}$ are translational and angular acceleration vectors, $\mathbf{g}$ is the gravitational acceleration, $\mathbf{F}_c$ and $\mathbf{M}_c$ are the force and the torque caused by all contacts on the particle, and $\mathbf{F}_{ext}$ and $\mathbf{M}_{ext}$ are force and torque resulting from other extenal forces such as hydrodynamic forces. Therfore, given the contact interaction laws, particles displacements evolution can be described through an appropriate time stepping integration of (Eqs. 1). The algorithm of computations for each time step is as follows: (1) The positions and the dimensions of particles are used to compute contact forces between each other and with boundary walls. (2) Particles accelerations are computed by means of the equations of motion (Eqs. 1) using contact and other external forces acting on

them. (3) The "velocity verlet" scheme is used for the integration of the equations of motion over a time step in order to calculate the particles displacements. (4) Particles positions are updated according to the calculated displacements.

For the sake of simplicity, particles are assumed in this work to be spherical in 3D modeling and circular in 2D modeling. The contact force $\mathbf{F}_c$ between two particles i and j is decomposed into two components, a normal part $\mathbf{N}_c$ and a tangential part $\mathbf{T}_c$ due to friction between particles. For the normal force law, we use a linear-elastic approximation; $\mathbf{N}_c = \left(-k_n\delta + 2\alpha\sqrt{mk_n}\dot{\delta}\right)\frac{\ell}{\|\ell\|}$ if $\delta < 0$, otherwise $\mathbf{N}_c = \overrightarrow{0}$. Here ℓ is the branch vector, it is expressed in terms of the position vectors of the grains $\ell = \mathbf{x}_{pj} - \mathbf{x}_{pi}$, δ is the gap or the overlap between the two contacting particles; $\delta = \|\ell\| - \frac{1}{2}(d_i + d_j)$ where d_i and d_j are the particles diameters, k_n is the normal stiffness, $m = \frac{m_i m_j}{m_i + m_j}$ is the reduced mass and $\alpha \in [0, 1[$ is a damping parameter which controls energy dissipation due to inelastic collision. For the friction, we use the classical Coulomb law expressed as a nonlinear relation between the friction force $\mathbf{T}_c$ and the sliding velocity vector $\boldsymbol{\delta}_t$ with a viscous regularization around the zero velocity; $\mathbf{T}_c = \min\left\{\beta\left\|\dot{\boldsymbol{\delta}}_t\right\|, \mu_f\|\mathbf{N}_c\|\right\}\frac{\dot{\boldsymbol{\delta}}_t}{\left\|\dot{\boldsymbol{\delta}}_t\right\|}$, where β is the tangential viscosity parameter and μ_f is the coefficient of friction. Similar force laws are used to compute the interactions of the grains with the plates boundaries (Richefeu *et al.*, 2006).

In order to describe the contact phase correctly, the time step of integration should be sufficiently small compared to the contact's duration Δt_c. This later could be estimated from the shosen normal stiffness k_n and the mass of the smallest particle m as $\Delta t_c = \pi\sqrt{m/k_n}$. The computation time step Δt used in simulations is usually taken less than a limite value

$$\Delta t_{DEmax} \approx 0.1\pi\sqrt{m/k_n} \qquad [2]$$

3. Lattice Boltzmann Method

3.1. *Standard formulation*

In the Lattice Boltzmann Method, one solves the kinetic equation for the particle distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$, in which $\boldsymbol{\xi}$ is the velocity vector, $\mathbf{x}$ the spatial position vector and t is the time. The macroscopic quantities of interest such as mass density ρ and momentum density $\rho\mathbf{u}$ are weighted averages of the distribution function; $\rho = \int f d\boldsymbol{\xi}$ and $\rho\mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}$. A popular kinetic model adopted for the method is the so-called BGK (Bhatnagar, Gross and Krook) model. In this model the collisions term in the Boltzmann equation is simplified using the simple relaxation time approximation

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi}.\boldsymbol{\nabla} f = -\frac{1}{\lambda}(f - f^{(0)}) \qquad [3]$$

where $f^{(0)}$ is the equilibrium distribution function (Maxwell-Boltzmann equilibrium function) and λ is the relaxation time. To solve for f numerically, Eq.(3) is discretized

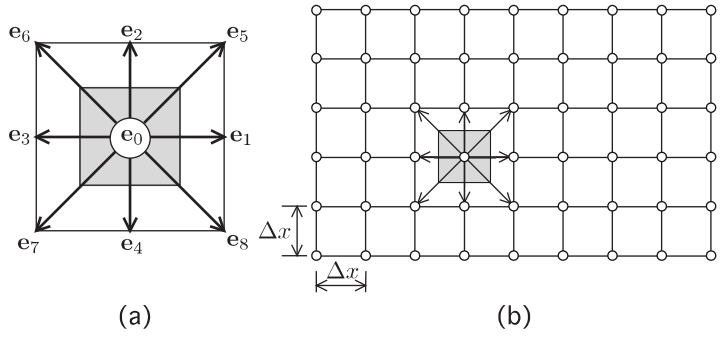

Figure 1. *(a) D2Q9 model, (b) Flow domain discretization using the D2Q9 model*

twice, a first discretization with respect to the time that is divided to increments Δt and a second one in the velocity space by chosing a finite set of velocity vectors that particles can have. The continuous particle distribution function $f(\mathbf{x}, \boldsymbol{\xi}, t)$ becomes therefore, a set of discrete distributions $f_i(\mathbf{x}, t)$ associated to the chosen velocity vectors $\mathbf{e}_i$. These discretizations lead to the LBGK (Lattice BGK) equation, that describes the incremental evolution of the discrete particle distributions f_i

$$f_i(\mathbf{x} + \mathbf{e}_i\Delta t, t + \Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{(eq)}(\mathbf{x},t)\right) \qquad [4]$$

where $f_i^{(eq)}$ is the discrete equilibrium distribution and τ is the dimensionless relaxation time, so that $\frac{1}{\tau} = \frac{\Delta t}{\lambda}$. In this way the mass and the momentum densities can be rewritten as sums; $\rho = \sum_{i=0}^{Q-1} f_i$ and $\rho\mathbf{u} = \sum_{i=0}^{Q-1} \mathbf{e}_i f_i$ where Q is the number of the chosen discrete velocity vectors.

As an illustration, we present in the following the widely used model in 2D simulations. It is named D2Q9 model (2 Dimensions, 9 Velocity vectors). Its discrete velocity vectors are chosen as follows (Fig. 1a). $\mathbf{e}_0 = c(0,0), \mathbf{e}_1 = c(1,0), \mathbf{e}_2 = c(0,1), \mathbf{e}_3 = c(-1,0), \mathbf{e}_4 = c(0,-1), \mathbf{e}_5 = c(1,1), \mathbf{e}_6 = c(-1,1), \mathbf{e}_7 = c(-1,-1), \mathbf{e}_8 = c(1,-1)$, where c is the characteristic velocity of the model. In this way Eq.(4) describes the incremental evolution of the discrete particle distributions f_i in nodes of a regular lattice having a space step $\Delta x = c\Delta t$ (Fig. 1b). The equilibrium distribution in its discrete form is $f_i^{(eq)} = \rho w_i \left[1 + \frac{3}{c^2}\mathbf{e}_i.\mathbf{u} + \frac{9}{2c^4}\left(\mathbf{e}_i.\mathbf{u}\right)^2 - \frac{3}{2c^2}\mathbf{u}.\mathbf{u}\right]$ whith w_i are weighting factors; $w_0 = 4/9$, $w_{1,2,3,4} = 1/9$, $w_{5,6,7,8} = 1/36$.

The discrete density distributions f_i are calculated at each time step according to Eq. (4) in two steps;

collision step: $f_i^{out}(\mathbf{x},t) = f_i(\mathbf{x},t) - \frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{(eq)}(\mathbf{x},t)\right)$

streaming step: $f_i(\mathbf{x}+\mathbf{e}_i\Delta t, t + \Delta t) = f_i^{out}(\mathbf{x},t)$

where f_i^{out} represents the post-collision density distribution.

After the streaming step the discrete distributions f_i are obtained in all nodes, consequently the mass and momentum densities can be calculated at each node. The fluid pressure p can be computed from the mass density through the equation of state $p = c_s^2 \rho$, where c_s is the sound speed of the model given in terms of the lattice speed c as $c_s = c/\sqrt{3}$.

3.2. *Discretization parameters for incompressible fluid flow simulations*

It can be shown through the Chapman-Enskog analysis (Luo, 2000) that LB models recovers the incompressible Navier-Stokes equation when the density fluctuation of the fluid is assumed to be negligible, where the equivalent kinematic viscosity is

$$\nu = \frac{1}{3} c \Delta x \left(\tau - \frac{1}{2} \right) \qquad [5]$$

Therfore, in order to correctly simulate an icompressible fluid flow, one must ensure that the density fluctuation is sufficiently small. This can be achieved using a model whose the sound speed c_s is sufficiently larger than the maximum velocity of the simulated flow u_{max}, i.e. the 'computational' Mach number defined as $Ma = \frac{u_{max}}{c_s}$ is sufficiently small. In practice, Ma should be maintained, smaller than 0.1. There are three model parameters Δx, Δt and τ. If given the viscosity of the fluid, only two of these parameters can be chosen independently since they are related through Eq. 5. In practice, it is often convenient to choose τ and Δx as two independent parameters and Δt is derived from Eq. 5. This is due to the fact that τ is largely responsible for the numerical stability of LB simulations and Δx is often dictated by the needed flow details in space. The BGK-LBM is convergent for $0.5 < \tau < \infty$. This range of τ corresponds to positive viscosities (Eq. 5). In practice τ is typically chosen in the range $0.5 < \tau < 3$.

3.3. *Solid moving boundary treatment*

Boundary conditions are introduced in LBM in terms of distribution functions f_i that are constructed from the imposed physical boundary conditions such as pressure and velocity. We present in the following the treatment of a solid moving boundary, since it is the principal one encountered in granular materials hydromechanics. Details about other boundary conditions in the LBM can be found in the literature. A simple way to represent solid obstacles such as solid particles in a LB dicretization, is to assume them as composed of grouped sets of pixels (voxels in 3D) whose centers are lattice nodes (Fig. 2). We call "fluid nodes" the nodes that are in the fluid domain and "solid nodes" the ones occupied by solid obstacles. A solid boundary node is a solid node having at least one link with fluid nodes. The fluid-solid interaction is done only through the boundary nodes. The interior solid nodes are useless in computation's process. It is assumed that there is no slip of the fluid on a solid surface, i.e. the fluid particles in contact of a solid surface have the same velocity as that of the surface.

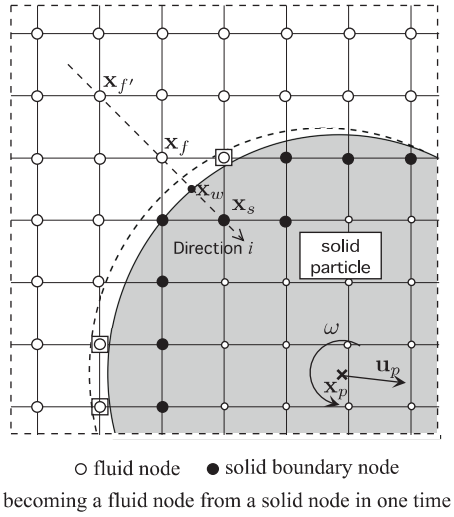

Figure 2. *Representation of a moving solid particle on a lattice grid*

This condition could be imposed in LBM using the bounce back scheme. This means that any incoming fluid particle from a fluid node to a solid node will be reflected back to the node it comes from. The momentum of the reflected particle may be different from the momentum of the streamed one, it depends on the position and the velocity of the solid boundary. Therfore, at the solid boundary nodes, instead of the collision step, the distributions that will be used in the streaming step are constructed using the post-collision distributions at neighboring fluid nodes. In this work we use the interpolated bounce back scheme proposed by Bouzidi et al. (Bouzidi *et al.*, 2001). For a linear interpolation, the post-collision distributions that will be assigned to solid boundary nodes before the streaming step are

$$\begin{cases} f_{\hat{i}}^{out}(x_s,t) = 2q f_i^{out}(x_f,t) + (1-2q) f_i^{out}(x_{f'},t) + 6 w_i \rho_w \frac{\mathbf{e}_{\hat{i}}.\mathbf{u}_w}{c^2}, & q \leqslant \frac{1}{2} \\ f_{\hat{i}}^{out}(x_s,t) = \frac{1}{2q} f_i^{out}(x_f,t) + \frac{2q-1}{2q} f_{\hat{i}}^{out}(x_{f'},t) + \frac{3}{q} w_i \rho_w \frac{\mathbf{e}_{\hat{i}}.\mathbf{u}_w}{c^2}, & q \geqslant \frac{1}{2} \end{cases} \quad [6]$$

where $\hat{i}$ refers to the opposite direction of the direction i ($\mathbf{e}_{\hat{i}} = -\mathbf{e}_i$), $q = \frac{\|\mathbf{x}_f - \mathbf{x}_w\|}{\|\mathbf{x}_f - \mathbf{x}_s\|}$ is a parameter defining the position of the solid boundary between the solid and the fluid node (Fig. 2), $\mathbf{u}_w$ is the velocity of the boundary and ρ_w is the fluid mass density at the boundary.

When a particle moves, there are grid nodes that move out of the solid region into the fluid region to become fluid nodes (indicated by □ in Fig. 2). Therfore one must specify some number of unknown distribution functions on this nodes. There are several techniques to compute values of the unknown distribution functions (on the

nodes which move from non-fluid to fluid region). In this model we use the simple technique described hereafter; unknown distributions are computed as the equilibrium distribution functions by using the averaged density in the system and the velocity of the solid particle at the specified node just before it leaves the the solid region.

3.4. *Hydrodynamic force on a solid particle, momentum exchange method*

Based on the bounce back scheme, the hydrodynamic forces acting on an obstacle can be obtained through the momentum exchange method. The momentum change of the bounced fluid particle is $(f_{\hat{i}}^{out}(\mathbf{x}_s,t)\times\mathbf{e}_{\hat{i}} - f_i^{out}(\mathbf{x}_f,t)\times\mathbf{e}_i)\times\Delta x^3$. Then, the average force transmitted over a time step Δt to the solid particle, along a boundary link k defined by boundary nodes $\mathbf{x}_f$ and $\mathbf{x}_s$ (Fig.2) is

$$\mathbf{F}_k = -\frac{\Delta x^3}{\Delta t}\left[f_{\hat{i}}^{out}(\mathbf{x}_s,t)\times\mathbf{e}_{\hat{i}} - f_i^{out}(\mathbf{x}_f,t)\times\mathbf{e}_i\right] \qquad [7]$$

Then the total hydrodynamic force exerted on the solid particle can be calculated by summing up the forces from all the related boundary links $\mathbf{F}_f = \sum_k \mathbf{F}_k$.

4. Coupling of DEM and LBM

In this model, coupling means the use of the DEM by introducing the hydrodynamic forces as external forces in the equations of motion of grains (Eqs. 1). These forces are obviously not independent of grains motion, therefore they should be re-evaluated continuously. The space LB discretization is dictated in this case by the diameters of the granular material particles. i.e. solid particles should be represented with a sufficient resolution. For moderate Reynolds numbers, the needed resolution to obtain an accurate evaluation of the hydrodynamic force is about 10 lattice across the diameter for a circular particle (2D) and about 7 lattice across the diameter for a spherical particle (3D). As mentioned above (Sect.3.2) the time step in LBM (noted in the follwing Δt_{LB}) depends on the other discretization parameters and derived from Eq. 5. Δt_{LB} is often larger than the maximum value for the DEM Δt_{DEmax} (Eq. 2). Therfore, one should perform a number n_d of DEM computation steps then perform one LB computation step, i.e. choose the DEM time step Δt_{DE}, such that $n_d.\Delta t_{DE} = \Delta t_{LB}$. The integer number n_d may be computed as $n_d = Int\left(\frac{\Delta t_{LB}}{\Delta t_{DEmax}}\right)+1$, then the DEM time step is set $\Delta t_{DE} = \frac{\Delta t_{LB}}{n_d}$.

5. Numerical applications

5.1. *Computation of permeability of a granular deposit*

A polydisperse granular sample with periodic boundaries in both horizontal directions is constructed using the DEM. The sample is then is subjected to an upward fluid

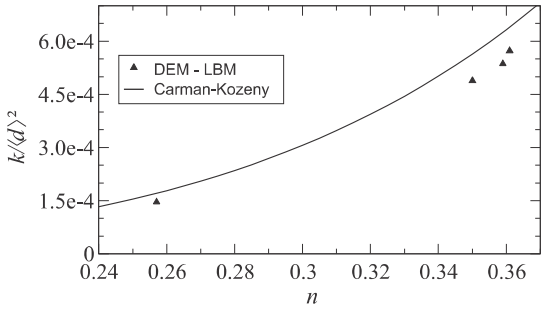

Figure 3. *Permeability vs. porosity.*

flow in order to measure its permeability, we use to this end the D3Q19 LB model. To drive an upward flow in the sample, the horizontal lower and upper boundaries are subjected to a pressure difference, we use the Zou & He (Zou *et al.*, 1997) pressure boundary conditions. In both horizontal directions periodic boundaries are implemented. Permeabilities are mesured for several samples having differentes porosities (noted n). All samples are composed of 200 spherical particles having diameters that follow the cumulative beta distribution (Voivret *et al.*, 2007)(with $d_{max} = 2d_{min}$). A comparison with the the permeability coefficient given by Karman-Kozeny formula is shown in (Fig. 3). The permeability coefficients are presented in a non-dimensional form $k/\langle d\rangle^2$ where $\langle d\rangle$ is the mean diameter of the sample grains. This graph shows that the variation of the permeability values obtained by numerical simulation has same shape as the Carman-Kozeny correlation. The differences between the DEM-LBM values and the Carman-Kozeny ones are for all points less than 15%.

5.2. *Assessement of the quick condition*

One of the samples described in Sect. 5.1 is subjected to an increasing hydraulic gradient. It is assumed that grains remain at rest until the boiling onset.The hydrodynamic forces on the grains of the sample are computed using the LBM, then injected in DEM to study the evolution of the vertical intergranular stress in a granular sample. The average vertical intergranular stress σ_{zz} is computed in five control slices, for each increment of the hydraulic gradient. Figure 4 shows the evolution of the normalized vertical stress in the centers of the five slices with increasing hydraulic gradient i. These stresses are obtained by dividing average vertical stresses by the vertical stress at the bottom of the sample σ^b_{zz}. It is clearly observable that the vertical stresses decrease when the hydraulic gradient increases. The critical value of the hydraulic gradient can be estimated as the point of intersection of the lines corresponding to the fives slices. In the present case, it is about $i_c = 1.040$. The critical hydraulic gradient is defined in classical soil mechanics as $i_c = \frac{(\rho_s - \rho_w)(1-n)}{\rho_w}$ where ρ_s and ρ_w are the solid and the fluid mass densities and n is the porosity. Using this expression for the

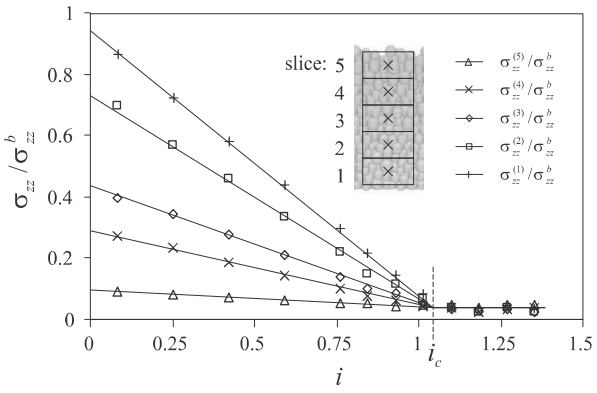

Figure 4. *Intergranular vertical stress vs. hydraulic gradient.*

sample's average porosity $n = 0.349$, leads to the critical hydraulic gradient value $i_c = 1.042$. Note that the sample's average porosity is obtained in our case numerically as the ratio of the fluid LB nodes to the total number of LB nodes in the model. It is clear that the obtained values of the critical hydraulic gradient with the numerical model and the classical formula are very close (1.040 and 1.042).

5.3. *Sedimentation of two particles "drafting, kissing and tumbling"*

The two validations performed above do not involve the effective DEM-LBM coupling since the solid particles are maintained at fixed positions with respect to the grid used by the LBM. In this application we simulate the sedimentation of two solid particles in a column of fluid. It is known experimentally that two particles dropped close to each other in a Newtonian fluid will undergo drafting, kissing and tumbling. For the sake of clarity in visualization, we perform a 2D simulation. The channel is $2\,cm$ wide (x-direction) and $8\,cm$ high (y-direction). The fluid has the properties of water with viscosity $0.01\,g/cm.s$ and density $1\,g/cm^3$. The particles density is $1.01\,g/cm^3$, and the radii of the particles are $0.1\,cm$. Initially, the first particle is $0.001\,cm$ off the channel center at a height of $7.2\,cm$ and the second particle is at the channel center at a height $6.8\,cm$. The two particles start settling in the y-direction, due to the gravity force.

Figure 5 shows the positions of the particles at different times. Fixed straigth lines on the particles are represented to show their rotations during the sedimentation. It is clear that the drafting, kissing and tumbling are well captured by the LBM-DEM simulation.

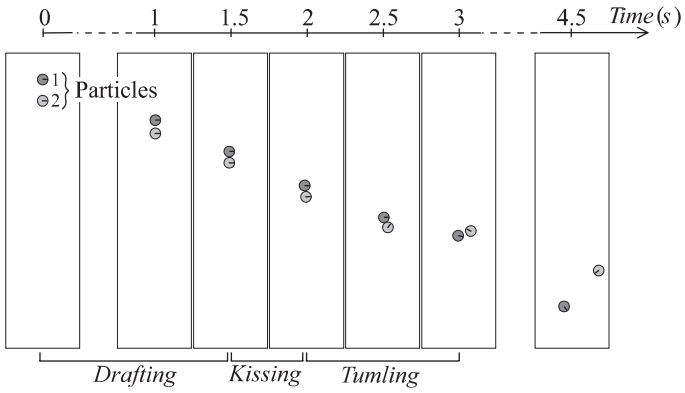

Figure 5. *Numerical simulation of two circular particles sedimentation at different time stages*

6. Conclusions

A 3D coupled DEM-LBM model is presented to investigate the micro-mechanical dynamic response of saturated granular materials. The first two numerical applications shown are made for the case of grains that are at rest, the obtained results are in good agreement with experimental results. For moving grains, The simulations show qualitatively correct results.

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