Use of Granular Material Dynamics Simulation for the Study of Cargo Shift of Ships

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ABSTRACT

In the current paper a modelling approach of granular material dynamics that can be interfaced with a ship motion model is described. Firstly, the existing simulation methods are critically assessed. Then, the adopted “discrete-particle” approach is described which is based on the so called “Molecular Dynamics” method. Some preliminary, yet characteristic, simulation results are produced, for a rectangular container vibrated in sway, in heave and in roll. The movement of cargo’s centre of mass is monitored. Critical parameter values (frequency, angle of tilt) for cargo shift and some preliminary comparison with the requirements of the international grain transport regulations are included.

Keywords: granular material, molecular dynamics, liquefaction

1. INTRODUCTION

Whilst the physical appearance of materials found in nature is quite varied, they can be classified under the four well-known states of matter: plasma, gas, liquid and solid. Yet experience suggests that some material cannot be put strictly under one category, because they bear the physical properties of two or more states of matter. Granular materials are ubiquitous in nature and yet they present high interest for the industry, being the second most manipulated material (Richard, 2005). Simply stated, by granular material is meant a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever these particles interact (Brown & Richards 1970). Despite their seeming simplicity, under different circumstances granular materials can exhibit substantial macroscopic differences in their behaviour. Subsequently, their handling often needs special attention. According to estimates, 40% of the capacity of many industrial plants are wasted because of problems related to the transport of these materials (Ennis et al., 1994). On the other hand, improvements in computational methods and resources in recent years have enabled significant progress internationally in the modelling of these materials that has led to better understanding of the behaviour of granular materials under a variety of excitations.

For naval architecture, the study of the behaviour of granular materials should be a topic of great interest, since cargo shift represents a major hazard for ship safety and probably the most common cause of capsize of large ships. However, the application of direct scientific modelling approaches for this important topic is basically non-existent. The current regulatory regime is governed by IMO’s Solid Bulk Cargoes Code [IMSB Code 268(85)] which however is prescriptive and largely empirical.

Recently there has been a spate of bulk carrier casualties with considerable loss of life, ostensibly initiated by the phenomenon known as “liquefaction”. As a matter of fact, liquefaction is a particularly dangerous issue since it turns what appears to be an apparently safe cargo like iron, nickel ore and core or sand slurry, into an easily movable cargo with a very detrimental effect on a vessel’s stability. The
ose body may behave like a liquid. In the current paper however, our focus is on the basic modeling of cargo shift phenomena, irrespectively of moisture. After a brief presentation of the existing simulation methods together with their limitations, in the following we describe a modelling approach that should lead, after interfacing with a ship motions model, to an integrated environment of ship – granular – material – dynamics investigation. A rectangular container is vibrated in roll, sway and heave and a preliminary identification of critical values for cargo shift is performed, taking into account international regulations’ requirements. It is believed that the simulation model can be a useful investigation tool before applying experimental methods.

2. RESEARCH PROGRESS

Notable names such as Coulomb, whose law of friction was originally stated for granular materials, Faraday, who discovered the convective instability in a vibrated container filled with powder, Reynolds, Hertz and others contributed to the body of research performed in this area. Brigadier Ralph Alger Bagnold was an early pioneer of the physics of granular matter and his book "The Physics of Blown Sand and Desert Dunes" remains an important reference to this day. Furthermore, various experimental works have been performed (an activity intensified in recent years) sometimes using quite sophisticated equipment. Wong et al (2005) used Positron Emission Particle Tracking to examine the quality of solids behaviour in vertically vibrated beds with heap formation, surface waves and arching. Sellerio et al (2011) studied experimentally the mechanical behaviours of granular materials submitted to forced vibrations, by the use of mechanical spectroscopy. Kawaguchi (2010) applied Magnetic Resonance Imaging to some dense granular flows or fluid-particle flows, such as the rotating drum, vibrated granular bed, hopper flow and spouted bed. His results confirm all the other observations.

In addition to experimental techniques, several theories have been applied for the handling of describing granular matter. In contrast to smooth particle dynamics method, where the continuum system itself is approximated by a discrete set of fluid particles, in the case of granular materials, continuum fields need to be constructed from discrete particle data. Specifically, these approaches are interested in deriving macroscopic fields, such as density, velocity and stress tensor from averages of microscopic variables such as the positions, velocities of, and forces on, each particle. In all these methods the important issue is to compute the continuum fields in the most appropriate way; that is to satisfy conservation laws. Among other approaches the coarse-graining approach (Goldhirsch, 2010) and the method of planes (Todd et al, 1995) are very popular. A general drawback for all these methods is that they are not universal (for every kind of grain) and sometimes they are leading to contradictory results because of the problems that they have near boundaries (Weinhart et al, 2012).

Despite, though, the great interest an overall coherent framework of granular materials investigation has not been fully set up yet. Scientific analysis refers mostly to a few prominent (primarily soil mechanics) problems. Performing similar research with relevance to ships is quite complex due to the dynamic nature of ship and cargo responses to random environmental excitations, the variety of transported materials substantially differing in properties and sizes, the presence of humidity etc. Nevertheless, with the vast computer power that is available today it seems that modelling work on this topic is possible.
3. EXISTING SIMULATION METHODS

Experiments with engineering devices are frequently expensive and sometimes even dangerous. Combined with the fact that there is no comprehensive theory on granular materials, numerical simulations can be used to reliably predict the behaviour of such materials for specific scenarios of container size, fullness, material type and size etc. Numerical simulations of interacting discrete media drive in the last twenty years an ever-growing interest in the granular microstructure and its link with macroscopic behaviour. Even by personal computers, sophisticated 2D or 3D systems of 20,000 particles can be simulated over a real time of a few seconds to a few minutes, offering the possibility to explore the effect of many parameters that would be hardly accessible by direct experimentation. Below is given a brief description of the most important simulation methods that are currently applied internationally:

3.1 Event-driven Molecular Dynamics

Molecular dynamics algorithms can be divided into two broad classes: those for soft and for hard bodies. The hard sphere modelling (event-driven molecular dynamics) is based on the absence of interpenetration or deformation during impact. It implies that velocities change according to the collision rule but the positions of the particles are the same before and after such an event. During the time intervals between collisions, the particles move along known ballistic trajectories. Therefore, the positions of the particles at the time of the next collision can be computed in one step. The calculation is purely algebraic because collisions are taken to the perfectly elastic: during a collision no energy is transferred either to deform or to change its internal state. The loss of linear momentum is characterized solely by means of the coefficient of elastic restitution, at least when rotations are neglected. In spite of its algebraic determinism, the algorithm produces phase-space trajectories that are chaotic, chaotic not only because of collisions, but also because of a delicate coupling among the algorithm, software and hardware. That’s why the simulation of granular gases is the main application of event-driven method. However the application of event-driven simulations is justified. Muller & Poschel (2012) showed that depending on the material and system parameters, the assumption of instantaneous events may fail.

3.2 Soft sphere Molecular Dynamics

The soft sphere approximation is based on an entirely different principle. Soft sphere Molecular Dynamics (called Molecular Dynamics from now on) plays the most important role among the simulation methods for granular systems. It is the time-dependent numerical solution of Newton’s equation of motion for all particles of which the granular material consists. This method allows us, in principle, to simulate systems of complicatedly shaped particles in dynamic and static situations, and also in the case of multi-particle contacts. Here friction and elastic restitution come into play when spheres penetrate into each other, and the magnitude of the interaction depends on the penetration depth. Such simulations have been proven to be very useful and predictive in many applications, in particular when the dynamical behavior of the grains dominates the system properties. Molecular Dynamics requires only one precondition: one needs to know the forces and torques acting between contacting particles as functions of the particles’ positions, their velocities, their angular orientation, and their angular velocities.

Although Molecular Dynamics provides an exact description of granular systems as the trajectory of each grain is computed, its application is restricted to rather small system size due to the time-intensive numerical solution of Newton’s equation of motion. Since Molecular Dynamics is the method used in this project for the simulation of granular dynamics an extended description of this method is given in the next part. Pioneering work in the field of Molecular Dynamics of granular materials has been done by Cundall (1979).
3.3 Direct Simulation Monte Carlo

The method of Direct Simulation Monte Carlo is intended to solve the Boltzmann or Boltzmann–Enskog equation, i.e., it determines the velocity distribution as a function of the spatial position \( r \) and time \( t \). This integration is performed by subjecting imaginary probability units \( \Delta f (r, t) \) to the action of the collision operator. Since the velocity distribution function represents the probability to find a particle in a certain phase space interval, in a sense, these probability units can be understood as quasi-particles.

Direct Simulation Monte Carlo, is more efficient than the event-driven method, although, further simplifying assumptions are required. The necessary precondition of uncorrelated motion of particles (molecular chaos assumption) is approximately valid for dilute granular systems, also called granular gases. As granular gases have been studied intensively by means of kinetic theory, Direct Simulation Monte Carlo is suited for direct comparison with the results of kinetic theory.

In addition, although the physical and mathematical basis of Monte Carlo may be less transparent to a novice that for molecular dynamics, Monte Carlo is usually easier than molecular dynamics to code in a high-level language such as C++. Monte Carlo is also easier than Molecular Dynamics to implement for systems in which it is difficult to extract the intermolecular force law from the potential function. Systems having this difficulty include those composed of molecules that interact through discontinuous forces; examples are the hard-sphere and hard convex-body models. Similar difficulties arise in systems for which the potential function is a complicated multidimensional surface, such as might be generated by ab initio calculations.

For determination of simple equilibrium properties such as the heat capacity, compressibility, and interfacial properties. Besides configurational properties, Molecular Dynamics also provides access to dynamic quantities such as transport coefficients and time correlation functions. Such dynamic quantities cannot generally be obtained by Monte Carlo, although certain kinds of dynamic behavior may be deduced from Monte Carlo simulations (Baumann, 1993). Molecular dynamics also offers certain computational advantages because of the deterministic way in which it generates trajectories. The presence of an explicit time variable allows us to estimate the length need for a run: the duration must be at least several multiples of the relaxation time for the slowest phenomenon being studied. No such convenient guide is available for estimating the length required for a Monte Carlo calculation. Finally many kinds of small errors in a molecular dynamics program tend to accumulate with time and so become apparent as violations of conservation principles; in contrast, subtle errors in a Monte Carlo program may not blatantly advertise their presence. As a result DSMC should be used with some care as inappropriate application may easily lead to non-physical results.

3.4 Rigid Body Dynamics

The idea of Rigid-Body Dynamics is complementary to the idea of Molecular Dynamics. While Molecular Dynamics simulations are always based on the evaluation of interaction forces, Rigid-Body Dynamics (sometimes also called Contact Dynamics) is based on the opposite idea: The interaction forces are determined from consistency requirements on the behavior of the particles. With much higher numerical effort Rigid-Body Dynamics allows for highly realistic simulation of systems comprising very stiff particles of complicated shape, which exhibit slow dynamics. However, as a direct consequence of disregarding material properties we have to sacrifice the uniqueness of the contact forces. Thus, the algorithm does not necessarily compute the physically-correct sets of contact
forces of a many-particle system, but one out of many (in general out of an infinite set of contact forces). Therefore, it cannot be assured that the system behaves in a physically-realistic way. Rigid-Body Dynamics has also been applied to granular systems, where frictionless smooth spheres have been simulated. A practical description of the application of Rigid-Body Dynamics to systems of spheres is presented by Unger et al (2002).

3.5 Other Methods

Besides the above mentioned there exists a number of further methods and algorithms for the simulation of granular systems. Some of these methods turn out to be significantly more efficient than the above mentioned ones, although they are restricted to certain types of problems. The most important further methods are Cellular Automata and bottom-to-top reconstruction which treat the system as a sequence of single particle problems (The algorithm may yield satisfactory results when treating systems where the boundary conditions change only very slowly. In such cases Molecular Dynamics is frequently inefficient).

4. OUR SIMULATION APPROACH

Our discrete-particle fluid model is based on the soft sphere Molecular Dynamics method. Granules are considered at this stage as smooth spherical particles with slightly different diameters (3 mm diameter with standard deviation 5%) that can translate or rotate in any direction. Furthermore, for the needs of this work we assume dry granular materials (granular solid and aggregate). The analysis is based on the C++ algorithm, described by Poeschel & Schwager (2005). We have chosen C++, instead of Fortran or some ready to use molecular dynamics simulator such as LAMMPS (also written in C++) and NAMD since the Standard Template Library (STL) provides structures (e.g. vectors and sets) that allow for the implementation of complex algorithms at relatively low programming effort. As illustrated in Figure 1, Molecular Dynamics Simulation is associated with three tasks: developing a mathematical model, using the model in a simulation and analyzing the simulation results.

Model development, includes choosing a form for the potential (intermolecular and molecular – environment) and then deriving appropriate equations of motion in order to model individual particles. For our study, we consider nonlinear frictional forces that act normally and transverse to the line of contact during collisions as shown in Figure 2. For the normal force we adopt the dissipative Hertz-type force for viscoelastic materials presented by Brilliantov et al (1996):

$$F_n = -k_n \dot{\xi}^{3/2} - \gamma_n \dot{\xi}^{1/2} \dot{\xi}$$  

(1)
where $\gamma_n$ is a damping constant connected to the radii of the spheres and the coefficients of bulk viscosity. $k_n$ is a non-linear stiffness of a spring whose elongation is $\zeta (\zeta = \max (0, R_1 + R_2 - |r_2 - r_1|))$, the deformation of the grain, connected to the elastic properties (Young Modulus, Poisson ratio) and to the radii of the spheres. For the transverse force we adopt the model proposed by Haff & Werner (1986):

$$F_t = -\min(|\gamma, u, |, |\mu F_n|) \cdot \text{sign}(u)$$  \hspace{1cm} (2)

Here $\gamma_s$ is a shear damping constant without physical interpretation, $u_s$ is the shear velocity component and $\mu$ stands for the dynamic friction coefficient. Since we consider only isolated systems, the equations of motion are simply obtained from Newton’s second law. Thus the problem is reduced to the integration of Newton’s equations of motion for the translational and rotational degrees of freedom.

The force $F_i$, the torque $M_i$, which act on particle $i$ of mass $m_i$ and the moment of inertia $J_i$, are functions of the particle positions $r_j$ and their angular orientations.

Trajectory generation refers to movements’ simulation of a large number of the model particles and divides into three major parts: initialization, equilibration and production. Of the large number of finite-difference methods that can be devised we use an efficient predictor-corrector method introduced by Gear (1971) which has proven to be powerful for Molecular Dynamics, because of its numerical stability. In specific Gear algorithm predicts molecular positions at time $t+\Delta t$ using a fifth order Taylor series based on positions and their derivatives at time $t$, evaluates the force on each grain at time $t+\Delta t$ using the predicted positions and Newton’s 2$^{nd}$ law and finally correct the predicted positions and their derivatives using the discrepancy between the predicted acceleration and that given by evaluated force. To gain computational time efficiency a Neighbour List algorithm (Verlet, 1967) is introduced. For each grain $i$, the method maintains a list of neighboring grains that lie within a predefined distance of $i$. As a result the list identifies those grains that contribute to the force on grain $i$.

To gain result analysis; that is reliability analysis of computed trajectories, analysis of simulation data for the required collective phenomenon and visualization of trajectories, we use the software package Paraview 3.12 (Sawley et al, 2007). ParaView is an open-source, multi-platform application for the visualization and analysis of scientific datasets, primarily those that are defined natively in a two- or three-dimensional space including those that extend into the temporal dimension. The front end graphical user interface (GUI) has an open, flexible and intuitive user interface that still gives you fine grained and open ended control of the data manipulation and display processing needed to explore and present complex data as you see fit.
5. SIMULATION RESULTS

For the purpose of our work we consider a mobile, rectangular, smooth and rigid tank, filled partly by dry granular material. The origin of the coordinate system is placed at the left side of tank’s bottom (Figure 3). Tank is free to move in any possible direction. Following Schafer et al (1996), our tank walls are built of particles to model surface roughness. Motion of the walls is prescribed and it can be periodic or random. In this specific application the model consists of 2,200 particles of which approximately 1800 can move relatively to the tank (the rest are wall particles). Tank length and height are denoted by \( l \), \( h \) and for our case their values are 19.2 and 6.4cm, respectively. In order to facilitate the validation of our code by comparing some of the results directly with experimental data given by Drake (1991) and Forester (1994), we use a specific granular material, namely the cellulose acetate spheres of mass \( 1.48 \times 10^{-4} \) kg.

Table 1: Numerical values for particle coefficients.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (mm)</td>
<td>3 ± 5%</td>
</tr>
<tr>
<td>Mass (kg)</td>
<td>1.48 x 10^{-4}</td>
</tr>
<tr>
<td>Poisson ratio</td>
<td>0.28</td>
</tr>
<tr>
<td>Young modulus (N/m^2)</td>
<td>3.2 x 10^9</td>
</tr>
<tr>
<td>Coulomb friction (( \mu ))</td>
<td>0.25 ± 0.02</td>
</tr>
<tr>
<td>Shear damping (( \gamma ))</td>
<td>20 Nsec/m</td>
</tr>
</tbody>
</table>

* Cellulose acetate particles

Even though our model could be used to simulate any realistic external oscillation (e.g. sea waves), we assume prescriptive periodic external excitation of the form \( n_1 \sin(2\pi f_1 t) \), where \( n_1 \) and \( f_1 \) are horizontal excitation’s amplitude and frequency, respectively. By giving to \( n_1 \) a constant value (10cm) we are able to test system’s behaviour under various excitation frequencies. Figure 4 presents a tank snapshot when \( f_1 = 2Hz \) (Figures 4 to 9 are presented at the end of the paper). One second after the excitation begun, the free surface started to behave like a liquid surface. Figure 5 presents the horizontal (left) and vertical (right) movement of the mass center when the system oscillates under five different excitation frequencies. As it is shown, for \( f_1 = 0.2Hz \) the mass centre is practically insensitive, in both the \( y \) and \( z \) directions. This implies that the particles follow the movement of the tank. As the frequency increases the mass centre starts to oscillate both along the \( y \) and \( z \) axes with a period close to that of the external excitations period. As expected, under a high frequency external excitation the free surface moves almost like a fluid and patterns of high amplitude waves are produced. An interesting point of observation is that the mass centre does not remain at the middle of the tank, as was expected, but it is shifted by about 2cm along the \( y \) and \( z \) axes. This is due to the distribution inhomogeneity of particle diameter and the gaps that exist between them.

![Figure 3: The origin of the coordinate system is placed at the left side of tank’s bottom.](image)

5.1 Sway

We monitored the movement of the mass centre of the granules inside the tank, under sway oscillation. Furthermore, in order to have direct visual observation of the behaviour, we animated the whole movement of the system (this is the most time consuming step and the reason that we restrict our investigation only to the first seconds of the movement).
5.2 Heave

Thinking in the same way as for the sway oscillation and assuming periodic external excitation of the form \( n_3 \cdot \sin(2\pi f_3 \cdot t) \), where \( n_3 \) and \( f_3 \) are vertical excitation's amplitude and frequency, respectively, behaviour was tested under various excitation frequencies (as was the case for \( n_1, n_3 \) has a constant value of 10 cm). In Figure 6 is shown a snapshot of system’s behaviour for \( f_3 = 2Hz \). In a short while the free surface started moving in the horizontal direction. As it is shown in Figure 7, where the horizontal (left) and vertical (right) movement of the mass centre under various excitation frequencies is presented, the mass centre of the system for small excitation frequencies follows the movement of the tank. However a small oscillation of the mass centre along the \( z \) axis exists, in contrast to what is happening in the \( y \) axis where the mass centre appears as practically fixed. Nevertheless, for an excitation frequency \( f_3 = 2Hz \) the mass centre starts to oscillate both along the \( y \) and \( z \) axes. This means that, there is a critical value of frequency, after which a wavy free surface occurs. Once again, due to the distribution inhomogeneity of particle diameter and of gaps between them, the mass centre is not at the middle of the tank, as one would have expected, but it is shifted by about 2 cm along the \( y \) and \( z \) axes.

5.3 Roll

According to IMO’s Solid Bulk Cargoes Code [IMSB Code 268(85)], solid bulk cargoes should be classified, where appropriate, in accordance with the UN Manual of Tests and Criteria, part III. The various properties of a solid bulk cargo need to be determined, as required by this Code. Among other cargo information required, one should determine the angle of repose; that is the maximum slope angle of non-cohesive (i.e. free-flowing) granular material. It is measured as the angle between a horizontal plane and the cone slope of such material. The angle of repose is a characteristic of non-cohesive bulk cargoes. It is indicative of cargo stability and it establishes which provisions of the Code apply. The recommended test method is the tilting box method which is suitable for non-cohesive granular materials with a grain size not greater than 10 mm. A box (600mm long, 400mm wide and 200mm high) is filled with the material to be tested and the tilting system (rate of tilting should be approximately 0.3°/s) is then activated and stopped when the material just begins to slide in bulk.

We tested the response of the free surface under different rates of tilting. It was found that the model seems to predict the group of angles of repose in which the material can be classified (<20°, between 20° and 30° or > 30° etc.). For the considered material (cellulose acetate) the angle of repose is close to 15°. Hence, it belongs to the “below 20°” group of materials and it has to be handled diligently. However, for the prediction of the exact angle of repose one needs to handle effectively the shape of the initial surface which is currently receiving our detailed consideration. In Figure 8 are presented three time instants of the tilting tank, with rate of tilt 1.2°/s. As shown, the free surface is practically not moving till the angle takes a critical value. From this point the grains begin to flow. In Figure 9 the movement of the mass centre for two different tilting rates is presented. The left diagram corresponds to a rate of 17.2°/sec and the right diagram to a rate of 1.2°/sec. The interesting result is that both rates produce almost the same angle of repose. An explanation for this is that, both the tank and the angle of cellulose acetate with diameter 3 mm are quite small. However for smaller rate the results are more distinct; that is the exact point of the angle of repose is represented by a big step in the curve. It is expected that, for different material and tank sizes the two rates may produce angles with a larger difference.

6. CONCLUDING REMARKS

In the first part of this paper the existing methods of simulation of granular material behaviour, together with their limitations, were
discussed. In particular, the so called molecular dynamics (soft sphere) method, which is the basis of our investigation, was presented in detail. Starting from the properties of the elementary granules that make up the material of interest (in this case cellulose acetate; however other materials more relevant to transported ship cargo in bulk are also currently considered) and by incorporating their mutual interactions, we have built a simulation model. Attention was paid the model to be general enough so that to be capable to predict the behaviour of a real granular cargo in a variety of situations. The simulation model is currently considered for interfacing with a ship motions model. In the current report we restricted our scope in the case of prescribed harmonic external excitation.

Some first simulation results for a rectangular container vibrated in roll, sway and heave, were presented. Experimental reproduction of the results is currently underway and it will provide more confidence on the practical applicability of the method. Of course after experimental validation of results, the method will be used for materials relevant to ship cargo.

Figure 4: Different time moments (0, 1.6 and 3 s, left to right) for sway vibration at 2Hz.

Figure 5: Horizontal (left) and vertical (right) movement of the mass center under sway vibration.

Figure 6: Different time moments (0, 1.6 and 3 s, left to right) for heave vibration at 2Hz.
Figure 7: Horizontal (left) and vertical (right) movement of the mass center under heave vibration.

Figure 8: Different time moments (12, 14.3 and 17 s, left to right) for roll excitation.

Figure 9: Horizontal movement of the mass center under roll excitation for $17.2^{0}/s$ (left) and $1.2^{0}/s$ (right) tilting rate.

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