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Steepest descent ballistic deposition of complex shaped particles

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ABSTRACT

We present an efficient event-driven algorithm for sequential ballistic deposition of complex-shaped rigid particles. Each of the particles is constructed from hard spheres (typically $5 \ldots 1000$) of variable radii. The sizes and relative positions of the spheres may mutually overlap and can be chosen such that the surface of the resulting particle appears relatively smooth. In the sequential deposition process, by performing steps of rolling and linear motion, the particles move along the steepest descent in a landscape formed by the boundaries and previously deposited particles. The computer time for the simulation of a deposition process depends on the total number of spheres but only weakly on the sizes and shapes of the particles. The proposed algorithm generalizes the Visscher–Bolsterli algorithm [1] which is frequently used for packing of spheres, to non-spherical particles. The proposed event-driven algorithm allows simulations of multi-million particle systems using desktop computers.

1. Introduction

The numerical description of sedimentation processes of particles on a flat or curved surface under the action of gravity or another external force, is essential for the understanding of a wide range of phenomena. Therefore, efficient algorithms for sedimentation processes are needed. Among others, processes such as filtration, e.g. [2], various types of size segregation phenomena [3–5] and the structure of certain types of packing have been investigated, e.g. [1,6–10]. While the latter application is certainly the most important evidenced by an enormous body of literature, we wish to point out, however, that the general problem of packing, that is, arranging objects in a confined space, frequently aiming to highest density, is related but not identical to the problem of sedimentation. Similarly, the corresponding simulation methods, referred to as *packing algorithms* cover a much wider field than simulation of sedimentation, see comprehensive reviews on packing, e.g. [11,12] and packing algorithms, e.g. [13–15].

Early literature describes mainly sedimentation algorithms for monodisperse or polydisperse spheres due to simplicity of contact detection for spheres. However, obviously particle shape has an important effect on the packing structure and, thus, the physical properties of sediments, therefore, there is a need for simulations of non-spherical particles. Sedimentation of non-spherical particles was investigated by several authors using different particle models such as ellipsoids [16,17], spherocylinders [18,19], polygons (in 2d) [20,21] or polyhedrons [22] representing sharp edged particles and pixel or voxel descriptions of the particles [23], for a review see [15]. Of particular interest for the simulation of non-spherical particles

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are *multisphere models*, e.g. [24–27], where each particle is represented by a set of monodisperse or polydisperse spheres. Similarly as for spheres, contacts of such particles can be easily detected. On the other hand, by appropriately choosing the radii and relative positions of the constituting spheres, a multisphere particle can approximate any desired shape to arbitrary accuracy, provided the set of spheres is large enough. Therefore, the multisphere model compromises between numerical efficiency and realistic particle shape.

The dynamics of non-spherical particles in sedimentation processes follows Newtonian mechanics which is approximately solved numerically by Molecular Dynamics, e.g. [17,28], but also other techniques have been applied, such as Monte Carlo methods [23,16,18,29] and others [15]. A class of simulation methods particularly adopted to the problem of sedimentation of particles in gravity is referred to as *drop and roll algorithms* or *steepest descent ballistic deposition algorithms* (SDBD). There are three paradigms behind these algorithms going back to the pioneering work by Vold [30]: (a) the particles are deposited sequentially, one after the other; (b) the particles obey overdamped dynamics, along the steepest descent with respect to gravity in the landscape shaped by previously deposited particles and the container walls until the particle reaches a (meta-) stable position where the particle is deposited; (c) once deposited, the particles do not change their position. This algorithm was first described by Visscher and Bolsterli [1], and is discussed in detail in [31–33].

Following the path of steepest descent implies a sequence of motion of different type: the particle may (i) fall vertically, (ii) roll in contact with one other particle or (iii) roll in contact with two other particles. Changes of the type of motion correspond to changes of the number of contacts of the particle considered. The great advantage of SDBD is that its dynamics may be described as a sequence of discrete events [34], where the events correspond to the change of the type of motion. Therefore, SDBD can be simulated by event-driven algorithms, which are by orders of magnitude faster than by integrating Newton's equation of motion in Molecular Dynamics allowing for simulations of large systems, needed for statistical analysis of packings (see [8] for a simulation of up to 2.5×10^7). There exist different strategies to optimize the efficiency of SDBD-algorithms [33].

Unlike Molecular Dynamics, SDBD is not a universal algorithm for the dynamics of particle systems as it neglects the inertia of particles (see, e.g. [8]). Nevertheless, it has been successfully applied to a wide range of problems in physics and engineering, such as microstructure modeling of fuel cells [35], charge stabilized colloids [36], packings in pebble bed reactors [37], nano-structured materials [14], metallic glasses [38], problems in additive manufacturing [39], processing of minerals [40], microstructure of ash deposits [41,42], sintering [43], microstructure of reaction-sintered ceramics [44], porous media [45,46] and many others.

2. Steepest descent ballistic deposition of aggregates

By now, the literature covers only SDBD algorithms for mono- and polydisperse spheres and simple non-spherical particles such as ellipsoids or rods [47,48]. Realistic particles are, however, frequently of more complex shape, therefore, in this papers we describe an efficient and robust SDBD algorithm for the sedimentation of complex-shaped particles. Following the basic idea of multisphere particles frequently used in Molecular Dynamics simulations, the particles considered here are rigid aggregates of polydisperse spheres arranged in overlapping or non-overlapping relative positions. This algorithm presented here was applied in numerical investigations of the packing properties in agglomerates of nano-powders [10] (for a 2d version see [9]).

Fig. 1 shows examples of complex shaped particles also termed aggregates in the following. By choosing appropriate radii and relative positions (overlapping or non-overlapping) of the constituting spheres, different shapes can be modeled. Fig. 1(a) shows a rod-shaped particle consisting of 11 equal overlapping spheres, Fig. 1(b) shows a particle composed of 4 equal rods having in total 17 overlapping spheres, while Fig. 1(c) shows an agglomerate of 790 non-overlapping spheres as used in a simulation of packings of nano-particles [10]. Using multi-sphere method particle shape can be represented with high precision, e.g. Fig. 1(d) shows a particle composed of 1785 spheres, Fig. 1(e) shows a particle with 2520 spheres, and finally the particle in Fig. 1(f) has 6241 spheres.

While in most practical applications complex particles are modeled as aggregates of overlapping polydisperse spheres, in the following illustrations for the sake of clearness, we will sketch aggregates of non-overlapping equal sized spheres. The presented algorithm is, however, not restricted to this case.

The algorithm for steepest descent ballistic deposition of sphere aggregates presented here preserves the basic idea introduced by Visscher and Bolsterli [1] for simulations of the deposition of spheres: Particles are sequentially dropped and follow the path of the steepest descent on the surface of the landscape formed by the system boundary and by previously deposited particles. Once found a stable position in a local minimum, the particle is immobilized. Owed to the non-spherical shape of the particles, the motion along the steepest descent path is modified. First, it is not the center of a sphere which follows the steepest descent but the center of mass of the agglomerate and second, following the steepest descent, the dropped particle adopts slightly different modes of motion than described in [1], illustrated in Fig. 2. When not in contact with any other particle nor the container wall, the agglomerate moves vertically downwards, thus, following the steepest descent, Fig. 2(a). When having one contact, that is, one of the spheres constituting the aggregate is in contact with one sphere of the previously sedimented material or the wall, the aggregate rotates around an axis which is specified by the center of the immobile sphere and by the condition that the center of mass of the aggregate follows the steepest descent, see Fig. 2(b). When having two contacts, Fig. 2(c), the aggregate rotates around an axis specified by the centers of the