SIMULATION OF CONTACTING SPATIAL POLYHEDRAL PARTICLES

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Summary In the following, the collective dynamical behaviour of many convex and non-convex polyhedral bodies in space is described. To be able to simulate a high number of bodies, methods from Molecular Dynamics (MD) are frequently used. Here these methods are combined with collision detection methods and contact formulations adopted from Multibody Systems (MBS). The used methods are presented briefly and some simulation results are given.

MOLECULAR DYNAMICS

Originally in MD molecules are considered and it is the goal to describe their interactions and their collective behaviour. These interactions depend on macroscopic measurable properties of the materials, e.g. viscosity or elasticity. In such systems, where the dynamical behaviour is calculated on the scale of the molecules, a very high number of particles is investigated. In order to simulate such a high number of bodies, in MD the molecules are often modelled by rigid spheres, [1]. The material behaviour is then represented by the forces that are acting between the bodies. In MD such forces can be attractive forces like Van der Waals forces, but they can also be contact forces that are applied to a colliding molecule pair. To calculate the forces effectively, overlaps between the particles are accepted, and the value of the force depends on the distance between the colliding bodies. Such methods for the calculation of contact forces are also called constitutive methods, [7]. The constitutive laws from MD are here applied to three dimensional solid bodies of different shape. Another idea that is used in MD is the neighbourhood search. As the motion of a body depends on other bodies of the system, it is possible to search for close body pairs in advance and to evaluate the necessary force only between such body pairs. Different neighbourhood search methods have been developed, [1], and we compared some of the main methods, [2]. Here we want to use only the most efficient one for our applications, where the influence between the bodies is restricted to contacts only, [5], the Linked Linear List Method (LLL). In this method, neighbouring body pairs are determined before real collision detection is performed. Without such a neighbourhood search method, in the worst case, the number of necessary body pairs that have to be tested for collision is of $O(n^2)$. In order to check, whether bodies are close to each other, their positions are projected onto the system axes separately.

By means of LLL neighbouring body pairs are found by creating an overlap list for each axis. For each body the beginning and the ending of its projection are compared, and the order of these beginnings and endings is stored in the list. An overlap of two bodies along an axis is given, if there is a beginning or an ending of a body between the beginning and the ending of another body. In the next time step this list does not have to be created again. A linear behaviour of the simulation can be obtained, by investigating the almost sorted list of the old time step for changes in the order. Body pairs which are overlapping along all system axes are stored and these pairs then have to be checked for collision.

MULTIBODY SYSTEM DYNAMICS

Simulations of granular material or bulk solids are based on free bodies in space. In the space a free body has six degrees of freedom. Then, the equations of motion can be obtained easily taking into account three elementary rotations for example the Kardan-angles and three translational degrees of freedom, summarised in the vector $\mathbf{y}_i$, for every body i.

$$m_i \mathbf{H}_{Ti} \cdot \ddot{\mathbf{y}}_i = \mathbf{f}_i ,$$

$$\mathbf{I}_i \cdot \mathbf{H}_{Ri} \cdot \ddot{\mathbf{y}}_i + \mathbf{I}_i \cdot \dot{\mathbf{H}}_{Ri} \cdot \dot{\mathbf{y}}_i + \tilde{\boldsymbol{\omega}}_i \cdot \mathbf{I}_i \cdot \boldsymbol{\omega}_i = \mathbf{l}_i .$$

Here, $\mathbf{H}_{Ti}$ and $\mathbf{H}_{Ri}$ are the Jacobian matrices of translation and rotation of body i, respectively, m_i and $\mathbf{I}_i$ are the mass and the inertia tensor, $\boldsymbol{\omega}_i$ is the vector of angular velocity and $\mathbf{f}_i$ and $\mathbf{l}_i$ are the forces and moments acting on the body due to collision or other forces, [4]. After neighbouring body pairs have been found the time consuming collision detection for polygonal convex or non-convex bodies can be accomplished. In order to check, whether there is a collision between two neighbouring body pairs, it has to be checked, whether there is a vertex of one body inside the other body. We consider point P as a vertex of a body, which we want to check for collision with the star-shaped test body, compare Figure 1.

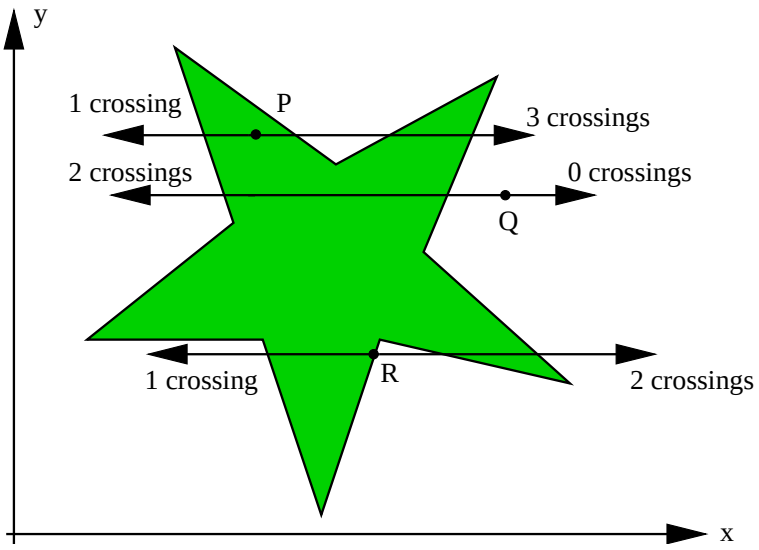

Figure 1: Collision Detection

Therefore, we define a ray from the observed point and another ray 180° rotated to it and count the intersections with the test body, [3]. In the planar case, point P is inside the other body, if the number of intersections with the surface of the other body is odd for the arbitrary ray, to both sides of the point. Also it can be said, that the point, e.g. point Q, is outside the other body, if the number of intersections is even for both rays (where we consider 0 to be an even number), and the point is positioned on the surface of the other body, e.g. point R, if the number of intersections is odd for on one side of the ray and even on its other side. For the spatial case the basic idea is the same but some more considerations have to be taken into account [3,6], and will be addressed in the talk. For the colliding bodies contact forces have to be computed. To apply the contact force to the bodies, the contact geometry has to be detected. For spherical bodies, the normal contact force simply acts in radial direction to the surface of the body. Here, more complex geometries are considered and the relevant surface part has to be found out. In the talk we want to line out, how we detect the contact geometry and how we compute the contact forces. The resulting forces and moments acting on each body must then be incorporated into the equations of motion given above.

RESULTS

The combination of MD and MBS makes it possible to simulate the dynamical behaviour of large systems of granular media consisting of arbitrary shaped bodies, as e.g. carriage systems. In the left part of Figure 2 a screw can be seen, where some bodies are moving down the winding. The right hand side of Figure 2 shows results of a different system that consists of spheres. In the figure a simulated system consisting of about 65000 bodies in space is shown. It can be seen, that it is possible to calculate quite large systems by combining both methods.

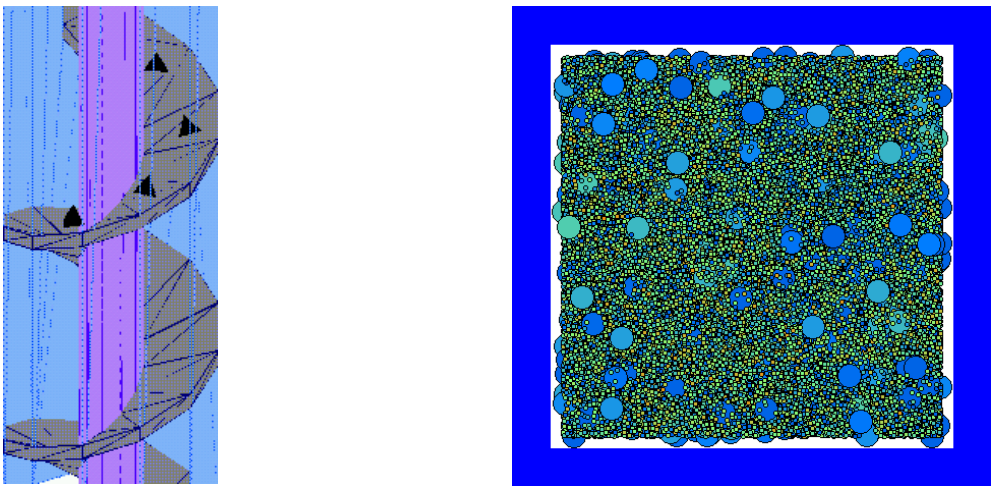

Figure 2: Results for polygonal and spherical bodies

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