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COLLISIONS OF PARTICLES IN LIMITED SPACE ANALYZED BY MOLECULAR DYNAMICS METHODS

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Abstract: Molecular simulations have received a great importance to model the properties and predict behaviors of solids, liquids and gases. The three-dimensional structural model of a material can be designed, in many cases, as a set of identical hard spheres occupying an available space. When this space is limited to a predetermined region, the properties of the material depend strongly on the arrangement and density of the particles; from this the scientific interest in the simulation of particle motions results. The consideration of collisions between particles in simulations is fundamental to obtain results, since the collisions represent a change of energy in the system, especially in deterministic methods such as Brownian dynamics, the general Langevin dynamics (which is an extension of Brownian dynamics), Monte Carlo methods (MC), discrete element method (DEM) and molecular dynamics (MD) (Haile, 1992).

Key words: Molecular dynamics, simulation, collisions, hard spheres.

Collisions are also associated with a wide range of applications such as robotics, car traffic safety, video games and other real-time animation systems, virtual and augmented reality, sensors, nuclear reactors, materials science, among others, where they appear in problems of the collision solution and prevention and treated by strategies for solving collisions using mathematical, physical or computational methods (Nanbu, 1980; Koura, 1990; Haile, 1992; Hubbard, 1995; Ericson, 2004; Tsou and Wayne, 2004; Je et al., 2009; Landau and Binder, 2009; Wang et al., 2012; Kala, 2016; Prasad et al., 2016; Capecelatro et al**.,** 2018) . Some of these systems can be interpreted as elastic collisions between hard spheres, and they are simulated by means of MD.

In the Chemistry area, processes are determined by the dynamic of collisions. Colloids are a good example, defined by the British encyclopedia as "any substance consisting of particles substantially larger than atoms or ordinary molecules but too small to be visible to the unaided eye". Some algorithms of molecular dynamics use periodic boundaries, in which the particles can move, instead of a restricted space (Haile, 1992). However, more realistic applications require algorithms to model collisions in closed spaces.

Given the importance of collisions in molecular simulations, the modeling of the collisions is necessary to determine and predict the behavior of the spheres. If the body is not an ideal sphere, it is possible to approximate its shape in this way: inscribing the body within the smallest sphere possible, similar to the idea proposed by Torquato and Stillinger in 2010.

In MD, the position of a sphere *i* is assigned in a deterministic manner according to the face-centered cubic structure (*fcc*). The velocities are first assigned using a uniform distribution and then are translated by a factor making the total linear momentum equal to zero (Haile, 1992), according to the formula $V_{xi}^{new} = V_{xi}^{old} - \frac{1}{N}\sum_{i}^{N} V_{xi}^{old}$ and similarly for the *y*- and *z*- axes. According to Tsou and Wayne (2004),

when two congruent spheres *i* and *j* having the radius *r*, the mass *m*, the position [*x*, *y*, *z*] and the initial velocity [*Vx*, *Vy*, *Vz*], collide, the modification of the trajectory and velocity are calculated for sphere *i* and *j*, according to the following expressions $V_{xi}^{new} = V_{xi}^{old} + \frac{J_x}{m}$ and $V_{xj}^{new} = V_{xj}^{old} - \frac{J_x}{m}$, respectively. The impulse J_x due to the normal force in the *x* direction at the moment of collision is $J_x = \frac{m\,\Delta x}{r^2}(\Delta \boldsymbol{V} \cdot \Delta \boldsymbol{r})$, one can use analogous expressions for the *y*- and *z*- components. Both particles follow the movements according to the new individual velocities until the next collision with another sphere or with a wall, and the trajectories continue to be updated throughout the simulation. The velocity of a sphere that hit the container wall is obtained by the following vector equation $\boldsymbol{V}_r = [\boldsymbol{V}_i \cdot \hat{\boldsymbol{p}}]\hat{\boldsymbol{p}} + [-\boldsymbol{V}_i \cdot \hat{\boldsymbol{n}}]\hat{\boldsymbol{n}}$; where $\boldsymbol{V}_r$ is a vector that indicates the new velocity of the particle *i*; $\boldsymbol{V}_i$ is the vector of the initial velocity of the particle, $\hat{\boldsymbol{p}}$ is a vector parallel to the wall of the cylinder, and $\hat{\boldsymbol{n}}$ is the vector of the normal to the particle moving direction before the collision at the point, where the particle hits the wall. When a sphere collides with a wall, there is no transfer of energy from the sphere to the wall, i.e., a sphere keeps the energy due to the considerable difference of the size. The vector of the normal calculation depends on the impact zone and the container geometry. The impact zone can be: 1) the lateral wall, 2) top and bottom walls, or 3) two or more walls simultaneously. The equations for these cases were developed, they are useful when a sphere impacts a single wall, but it is possible that a sphere hits the wall and one of the caps simultaneously. If this occurs, the line of movement of the particle is the same but the direction is opposite $\boldsymbol{V}_r = -\boldsymbol{V}_i$.

MD provides a methodology for detailed microscopic modeling at the molecular level, which is becoming an indispensable tool for both theoretic studies and applied researches (Xu and Li, 2015). The movement of spherical bodies under the action of a force field is the principle of the MD simulation; when a collision of a sphere with another sphere or with the wall occurs, the velocity is updated according to the momentum conservation law (Haile, 1992).

There are two natural approaches to simulate a system of particles: i) the event-driven simulation and, ii) the time-driven simulation. The former focuses on determination of the ordered sequence of particle collisions. In this model, all particles move in straight line trajectories at a constant speed between collisions. The latter discretizes the time into a number of periods of size *dt*; the position of each particle is updated every *dt* units of time and the overlaps between all particles are verified. If a collision has occurred, the position and the velocity of the particles are updated and the simulation continues.

In an MD modeling, there are two principal steps: 1) the development of model for the problem and 2) the simulation of MD applied to the model. The simulation is determined by the generation and analysis of the trajectories. The generation of the trajectories is made according to the type of the bodies that are being simulated and the permission of overlapping (hard or soft spheres); then the static and dynamic properties for received model are calculated.

The algorithms of an MD simulation are constituted by three stages: 1) *Initialization*, the initial structure is generated according to the face-centered cubic (*fcc*) lattice; the velocities are assigned to each particle according to Maxwell's distribution, causing the system to be in equilibrium; 2) *Equilibrium*. One of the main characteristics of this stage is that, regardless of the initial structure, the results of the simulation must be statistically equal. In this stage, the particles move indefinitely until the structure becomes disordered; this is measured by the parameter λ. The collision modeling is very important at this stage to reach the objective; and, 3) *Production*. In this last stage, the properties of the system are calculated; some equations to determine different static and dynamic properties are defined in terms of collisions.

A simulation of a hard-spheres system in a cylinder was developed using the fundamentals of MD and software MATLAB® to compute some structural properties: the atomic packing fraction (APF), the radial distribution function and the stats of the collisions during the simulation. The system simulated was colloidal silver, since in simulations of colloids the solute particles are considered to be hard spheres, and the presence of the solvent is not included into the MD calculations. In 2014, van Swol and Petsev established that this exclusion is correct when the solute–solute collisions predominate over the solute–solvent collisions.

The equations modeled were applied in the simulated system of colloidal silver. A simulation of a hard-sphere system in a cylinder in the software MATLAB® was developed using the fundamentals of

MD and the proposed equations to model collisions; some static properties of the system were computed: the *APF* represents the space occupied by atoms in the container, a material of a high *APF* is considered as a dense material, otherwise is a porous material; and the equilibrium structure of liquids and complex fluids in general is characterized by the radial distribution function *g(r)* (RDF), which is proportional to the probability of finding two atoms separated by the distance $r + \Delta r$ (van Swol and Petsev, 2014).The APF of the system was 0.2% and the frequency of collisions in the equilibrium stage was f_{eq}=2.2810.10^{3}Hz while for the production stage, it was f_{prod}=1.3995.105Hz. This model can be used not only for atoms/molecules that collide, but also for some rigid bodies. In a future work, particle collisions in irregular-shape containers will be modeled since in real systems, the channels are constricted spaces.

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