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COLLISIONS OF PARTICLES IN LIMITED SPACE ANALYZED BY MOLECULAR DYNAMICS METHODS

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Abstract. Goal. *The objective of this work is to propose a model that allows one to obtain velocity and direction of spherical hard-bodies after a collision, using Molecular Dynamics (MD) methods. Molecular simulations are employed to compute the properties and predict behaviors of solids, liquids and gases; the consideration of collisions between particles is fundamental, since they represent a change of energy in the system. Collisions are also associated with a wide range of applications such as robotics, car traffic safety, videogames, materials science, colloids, among others; some of them can be interpreted as elastic collisions between hard-spheres.* ***Problem.*** *Some algorithms of MD use periodic boundaries, in which the particles can move, instead of a restricted space. However, more realistic applications require algorithms to model collisions in closed spaces.* ***Originality.*** *Equations to model the collision in restricted spaces were developed to obtain the velocities of the spheres that collide with the wall(s) of the container; these formulas are valid when the walls are straight, for example in cylinders and cubes.* ***Methodology.*** *A simulation of a hard-sphere system in a cylinder was developed using the fundamentals of MD and the proposed equations to model collisions, in MATLAB. Properties of the system were computed: the atomic packing fraction (APF), which represents the space occupied by atoms in the container; and the equilibrium structure was characterized by the radial distribution function g(r) (RDF), which is proportional to the probability of finding two atoms separated by the distance $r + \Delta r$.* ***Results.*** *The APF of the system was 0.2%, and the frequency of collisions in the equilibrium stage was 2.2810×10^{3}Hz, while in the production stage was 1.3995×10^{5}Hz.* ***Practical value****-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.*

Key words**:** *Molecular dynamics, simulation, collisions, hard spheres, particle trajectory, distribution function.*

Introduction

Molecular simulations have received a great importance to model the properties and predict behaviors of solids, liquids and gases. A three-dimensional structural model of a material can be designed, in many cases, as a set of identical hard spheres occupying the available space. When this space is limited to a predetermined region, the properties of the material strongly depend on the arrangement and density of the particles; this implies a scientific interest in the simulation of the motion of particles in significantly limited volumes. The consideration of collisions between particles in simulations is fundamental to obtain results, since the collisions lead to a change in energy in the system, especially in deterministic methods, such as Brownian dynamics, general Langevin dynamics (which is an extension of Brownian dynamics), Monte Carlo methods (MC), discrete element method (DEM) and molecular dynamics (MD) [1].

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, material science, and others, where they appear in problems related to collision solutions and their prevention, and are treated by strategies for solving collisions using mathematical, physical or computational methods [1-12]. Some of these systems can be inter-

preted 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 Encyclopaedia as "any substance consisting of particles substantially larger than atoms or ordinary molecules but too small to be visible to the unaided eye" [13]. In 1995, Segre et al., evidenced that particles in suspensions of polymethylmethacrylate (PMMA) interacted like hard spheres [14]. The authors described accurate methods to determine both the particle radii and the sample concentrations, using Lattice-Boltzmann simulations, based on particle collisions. Efficient methods and devices, which used a collision analysis, have been developed for studying the size and configuration of colloidal particles, e.g. Rutherford scattering, mass spectrometer, ion beam analysis and electron microscope [8, 15-18].

Some algorithms of molecular dynamics use periodic boundaries, in which the particles can move, instead of a restricted space [1]. However, more realistic applications require algorithms to model collisions in closed spaces, when particles are located inside of a container and the collisions occur between particles as well as between particle and container walls.

In the present work, using the MD, a model has been developed for obtaining new velocities and directions when spherical hard-bodies collide with each other or against a straight surface. It then describes the MD simulation in the MATLAB for a hard-sphere system in a cylinder, and finally some concluding remarks are given.

Modeling of collisions between spherical objects

A collision determines the trajectory followed by a particle after chocking with another particle or a restricting surface. However, there exist a few algorithms that consider a restricted space of movements. Given the importance of collisions in molecular simulations, the modeling of the collisions is necessary to determine and predict the behavior of 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 [19]. The velocities assignment is as follows.

Velocity initializing

In any molecular simulation, the particles of a material are created with an initial position and velocity. In MC simulations, a sphere is randomly allocated according to a probability distribution function (PDF), usually a normal distribution or a Gaussian distribution [8]. 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 [1], according to the formula (1)

$$V_{xi}^{new} = V_{xi}^{old} - \frac{1}{N}\sum_{i}^{N} V_{xi}^{old} \qquad (1)$$

and similarly, for the *y*- and *z*- axes.

A model to assign these velocities is described below.

Interparticle collision

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 [V_x, V_y, V_z], collide, the modification of the trajectory and velocity are calculated according to the following expressions (2) and (3) [6]:

$$\text{Sphere } i\text{:}\quad V_{xi}^{new} = V_{xi}^{old} + \frac{J_x}{m} \qquad (2)$$

$$\text{Sphere } j\text{:}\quad V_{xj}^{new} = V_{xj}^{old} - \frac{J_x}{m} \qquad (3)$$

The impulse J_x due to the normal force in the *x* direction at the moment of collision is (4)

$$J_x = \frac{m\,\Delta x}{r^2}(\Delta \boldsymbol{V} \cdot \Delta \boldsymbol{r}). \qquad (4)$$

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.

Sphere-wall collision

In molecular simulations, the spheres are in constant movement being in an infinite space. However, if a simulation is considered in a restricted space such as a cylinder or a cub with straight walls is considered, the particles generate the proper trajectories in the container. The colli-

sions of a sphere with other spheres and also against the walls of the container can be modeled as follows.

The velocity of a sphere that hit the container wall is obtained by the following vector equation (5):

$$\boldsymbol{V}_r = [\boldsymbol{V}_i \cdot \hat{\boldsymbol{p}}]\hat{\boldsymbol{p}} + [-\boldsymbol{V}_i \cdot \hat{\boldsymbol{n}}]\hat{\boldsymbol{n}}\,, \qquad (5)$$

where

$$\hat{\boldsymbol{p}} = \frac{\boldsymbol{p}}{|\boldsymbol{p}|} \qquad (6)$$

$$\boldsymbol{p} = \hat{\boldsymbol{n}} \times \boldsymbol{A} \qquad (7)$$

$$\boldsymbol{A} = \boldsymbol{V}_i \times \hat{\boldsymbol{n}} \qquad (8)$$

As can be distinguished in fig. 1, $\boldsymbol{V}_r$ 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, as it is resumed in table 1. The impact zone can be: 1) the lateral wall, 2) top and bottom walls, or 3) two or more walls simultaneously.

The previous equations 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:

$$\boldsymbol{V}_r = -\boldsymbol{V}_i.$$

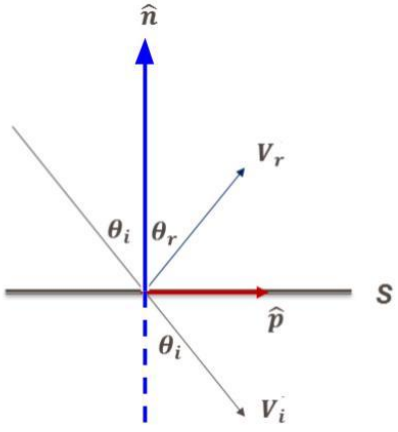


Fig. 1. Trajectory of a sphere after a collision with a straight wall

Simulation of a hard sphere system in a cylinder using MD

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 [20].

The movement of spherical bodies under the action of a force field is the principle of the MD simulation, which is considered as a deterministic model because the movement of each sphere is known. When a collision of a sphere with another sphere or with the wall occurs, the velocity is updated according to the momentum conservation law [1].

MD approaches

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 the 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 the 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. For better results, Leach (2001) suggests the time step durations with continuous potentials, according to the type of particles in the system, see table 2 [21]

In an MD modeling, there are two principal steps: 1) the development of a 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 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 the received model are calculated.

The objects can be modeled as hard spheres, bodies that do not represent any electric charge, and they cannot overlap each other. The molecular forces between these bodies are described by discontinuous functions of the distance between them. Namely, hard spheres exert forces on one another only in case of a collision.

Table 1 – Calculation of the vector of the normal for distinct containers and different impact zones

Geometry of the container	Impact zone	Vector of the normal $\hat{\boldsymbol{n}}$
Cylinder	Cylinder body	$\hat{\boldsymbol{n}} = \frac{-x_2\hat{\imath} - y_2\hat{\jmath}}{R}$
	Cylinder Caps	$\hat{\boldsymbol{n}} = \pm\hat{\boldsymbol{k}}$
Cube	Wall intersecting the *x*-axis	$\hat{\boldsymbol{n}} = \begin{Bmatrix} \hat{\imath}, if \quad x = r \\ -\hat{\imath}, if \quad x = L - r \end{Bmatrix}$
	Wall intersecting the *y*-axis	$\hat{\boldsymbol{n}} = \begin{Bmatrix} \hat{\jmath}, \quad if \quad y = r \\ -\hat{\jmath}, \quad if \quad y = L - r \end{Bmatrix}$
	Wall intersecting the *z*-axis	$\hat{\boldsymbol{n}} = \begin{Bmatrix} \hat{\boldsymbol{k}}, \quad if \quad z = r \\ -\hat{\boldsymbol{k}}, \quad if \quad z = L - r \end{Bmatrix}$

Table 2 – MD with continuous potentials: Time-step of the different types of movement present in systems

System	Movement type	Suggested time-step (in *s*)
Atoms	Translation	10^{-14}
Rigid molecules	Translation and rotation	5×10^{-15}

Simulation stages in MD

The algorithms of an MD simulation are constituted by three stages:

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.

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.

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. For example, the equation to calculate the compressibility factor is (10):

$$Z = 1 + \frac{md}{2E_k}\frac{1}{t}\sum_{c=1}^{N_c}\left|\Delta v_{ij}(t_c)\right|, \qquad (10)$$

where m is the mass and d is the diameter of the spheres, E_k represents the kinetic energy in the system, t is the lapse of time, N_c is the number of collisions, and v_{ij} is the change of velocity in the collision [1].

Results of the simulation

A simulation of a hard-sphere system in a cylinder was developed using the fundamentals of MD and the software MATLAB® to compute some structure properties: the packing fraction, the radial distribution function and the stats of the collisions during the simulation. The specifications of the computer used are: AMD A10 processor and a RAM of 16 GB, 800 MHz.

The simulated system was colloidal silver, since in the simulations of colloids, the solute particles are considered to be hard spheres, and the presence of the solvent is not included in 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 [22]. The parameters considered were taken from the characterization of colloidal silver dissolved in water, presented by Franco-Molina et al. [23]. The study was realized by dynamic light scattering (DLS); the solute showed a mean diameter of 100 nm.

The parameters of the simulated system are:

- Number of spheres N=225;
- Height of the cylindrical container L = 5;
- Diameter of the cylindrical container D = 2;
- The diameter of the spheres (particles of solute) d= 0.1 (equivalent to the size of 100 nm).

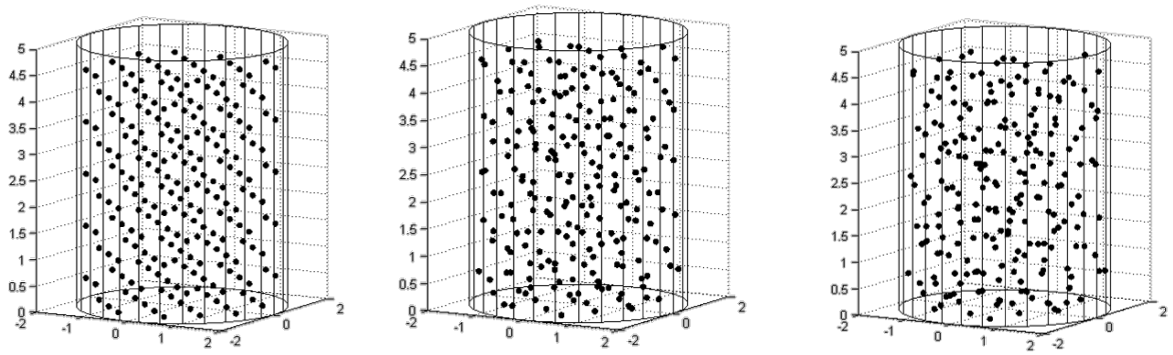
Atomic packing fraction

The atomic packing fraction (*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.

In the present simulation, the *APF* remains constant, and it is calculated by formula (11):

$$APF = \frac{V_{spheres}}{V_{container}} \quad (11)$$

According to Francon (1929), the importance of APF lies in the information that it provides about the structure of the material and the stability of its atoms [24]. Fig. 2 shows the stages of initialization, equilibrium and production of the simulated system.



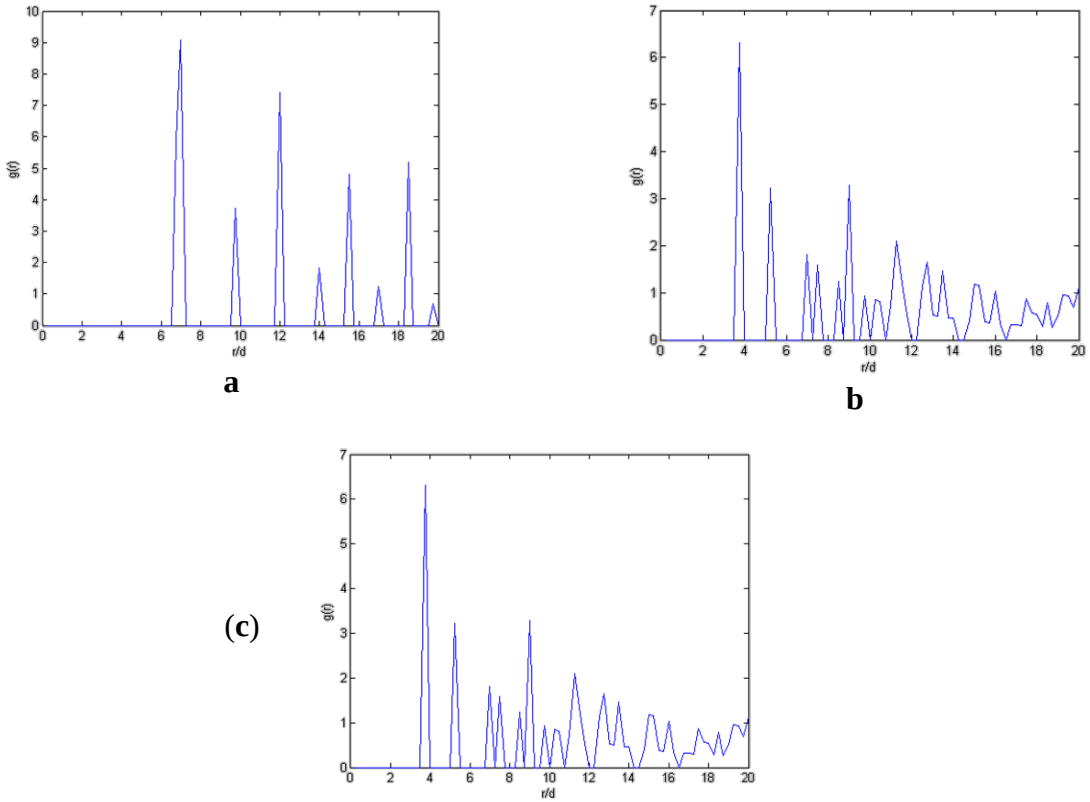
a b c

Fig. 2. Graphics of the MD simulation of colloidal silver in a cylinder, stages of: (a) initialization, (b) equilibrium, and (c) production (r=0.1, N=225 spheres, APF= 0.2 %)

Radial distribution function

The equilibrium structure of liquids and complex fluids in general is characterized by the radial distribution function *g(r)* (RDF). It is proportional to the probability of finding two atoms separated by the distance $r + \Delta r$ [22]. The RDF is calculated according to the equation (12) [25]:

$$g(r) = \frac{N(r,\Delta r)}{\frac{1}{2}N\rho V(r,\Delta r)} \quad (12)$$



a **b**

(**c**)

Fig. 3. The radial distribution function *g(r)* of the simulated structure in the stages of: (a) initialization, (b) equilibrium, and (c) production

Here $N(r, \Delta r)$ is the number of particles found in a spherical shell of radius r and thickness Δr, with the spherical shell centered on a fixed particle; ρ is the number density of the general system and $V(r, \Delta r)$ is the volume of the spherical shell.

The RDF indicates the influence of one particle in the system over the positions of the closest neighbors. In fluids, if the separation is less than one particle diameter, then $g(r)$=0; for large separations, the central particle does not influence the position of the others, then $g(r)$=1, this means that the density is uniform [1].

The graphs of the RDF of the stages from the simulated system are shown in fig. 3.

Analysis of the collisions

The equations modeled in previous section were applied in the simulated system of colloidal silver. The diagram in fig. 4 shows a comparison between the collisions sphere-sphere and sphere-wall in the stages of equilibrium and production. In the first stage, initialization, collisions are absent.

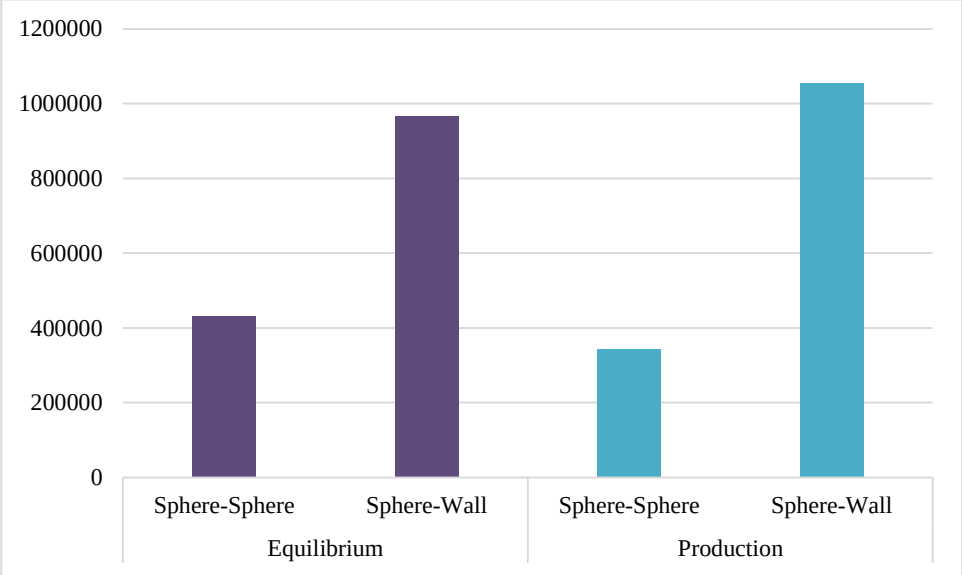


Fig. 4. Analysis of the collision in the MD simulation: stages of equilibrium and production

The simulation computed the frequency of collisions, resulting that the frequency of them in the equilibrium was $f_{eq}=2.2810\times10^{3}$Hz and, for the stage of production $f_{prod}=1.3995\times10^{5}$Hz.

Conclusions

In this work, the importance of the collision modeling in different areas of science and technology was evidenced.

Equations to model the collision in restricted (finite spaces) were developed to obtain the velocities of the spheres that collide with the wall(s) of the container. These formulas are valid when the walls are straight, for example in cylinders and cubes.

This model can be used not only for atoms/molecules that collide, but also for some rigid bodies.

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.

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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Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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ЗІТКНЕННЯ ЧАСТИНОК У ОБМЕЖЕНОМУ ПРОСТОРІ ПРИ АНАЛІЗІ МОЛЕКУЛЯРНИМИ ДИНМІЧНИМИ МЕТОДАМИ

Анотація. *Метою цієї роботи є запропонувати модель для отримання швидкості та напрямків, коли зіткнення сферичних твердих тіл здійснюється за допомогою молекулярної динаміки (МД). Молекулярне моделювання використовується для обчислення властивостей та прогнозування поведінки твердих речовин, рідин та газів; розгляд колізій між частинками є фундаментальним, оскільки вони являють собою зміну енергії в системі. Колізії також пов'язані з широким спектром додатків, таких як робототехніка, безпека автомобільного руху, відеоігри, матеріалознавство, колоїди та ін., деякі з них можна інтерпретувати як пружні зіткнення між жорсткими сферами. Деякі алгоритми МД використовують періодичні межі, в яких частки можуть рухатися, а не обмежене простору. Проте для більш реалістичних додатків потрібні алгоритми моделювання колізій у замкнутих просторах. Рівняння для моделювання зіткнення в обмежених просторах були розроблені для отримання швидкостей сфер, які стикаються зі стіною (контейнерами); ці формули справедливі, коли стіни є прямими, наприклад, у циліндрах та кубах. Симуляція системи твердіх сфер в циліндрі була розроблена з використанням основних принципів MD та пропонованих рівнянь для моделювання колізій в MATLAB. Знайдено властивості системи: фракція атомної упаковки (APF), яка представляє простір, зайнятий атомами в контейнері; і рівноважна структура характеризувалася функцією радіального розподілу g(r) (RDF), яка пропорційна ймовірності знаходження двох атомів, розділених відстані $r + \Delta r$. APF системи становила 0,2%, а частота зіткнень на стадії рівноваги становила $2{,}2810 \times 10^3$ Гц, тоді як на етапі виробництва $1{,}3995 \times 10^5$ Гц. Ця модель може бути використана не тільки для атомів / молекул, які стикаються, але також для деяких твердих тіл. У подальшій роботі зіткнення частинок у контейнерах з неправильною формою будуть моделюватися, оскільки в реальних системах канали є стисненими просторами.*

Ключові слова: *молекулярна динаміка, симуляція, колізія, тверді сфери, траєкторія частинок, функція розподілу.*

СТОЛКНОВЕНИЕ ЧАСТИЦ В ОГРАНИЧЕННОМ ПРОСТРАНСТВЕ ПРИ АНАЛИЗЕ МОЛЕКУЛЯРНЫМИ ДИНАМИЧЕСКИМИ МЕТОДАМИ

Аннотация. *Целью настоящей работы является: предложить модель для получения скорости и направлений, когда столкновения сферических твердых тел осуществляется с помощью молекулярной динамики (МД). Молекулярное моделирование используется для вычисления свойств и прогнозирования поведения твердых веществ, жидкостей и газов; рассмотрение коллизий между частицами является фундаментальным, поскольку они ведут к изменению энергии в системе.*

Ключевые слова**:** *молекулярная динамика, симуляция, коллизия, твердые сферы, траектория частицы, функция распределения.*