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Simulating Fluid Dynamics of the Alive Tissues with Brownian Motion

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Introduction

The aim of the current work is to create simulation model for fluid dynamics. Application of the method is for visualization of the movements of the molecules of the fluids in order to give physicians better understanding of the processes taking place in the human body.

Model

As a first step we will simulate thermodynamically state of the pure water.

Mathematical model that is used to model mutual influence of the molecules of water is taken from the [1]. It is called Lennard-Jones potential and is mathematical approximation that describes intermolecular interactions. The expression of the Lennard-Jones potential is given by the following equation:

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \qquad (1)$$

where ε – the depth of the potential well; σ – the distance at which the inter-particle potential is minimal; r – current distance between the two particles. The given equation follows closely the empirical measurements.

The term with the power of 12 describes intermolecular repulsion in short range due to overlapping of the electronic clouds. Its physical meaning comes from the Pauli principle which says that overlapping of the electronic clouds of the atoms increases the energy of the system abruptly.

The term with the power 6 describes the weak intermolecular forces between molecules as described in [2]. This is an attraction component and it has several sources. In our case for the water molecules it consists at least of electrostatic interaction between the water dipoles, the dispersion attraction also called London dispersion forces.

The graphical representation of the potential, according to the equation (1) is given on the Fig. 1.

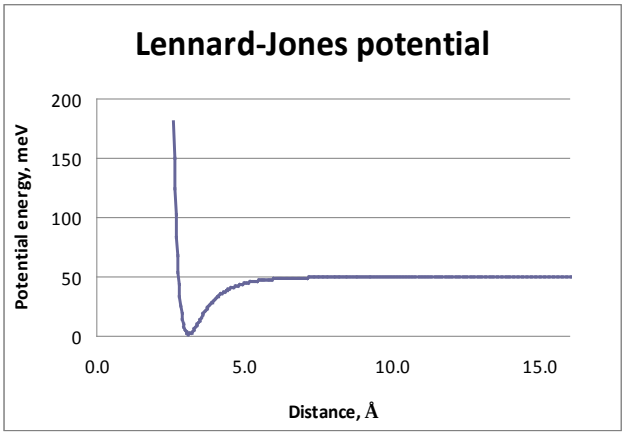

Fig. 1. Lennard-Jones potential

The actual resultant forces are obtained by differentiation of the equation (1) as follows:

$$F(r) = \frac{d}{dr}V(r) = 4\varepsilon\sigma^{6}\left(-12\sigma^{6}r^{-13} + 6r^{-7}\right). \qquad (2)$$

Their graphical representation as a function of distance is given on the Fig. 2.

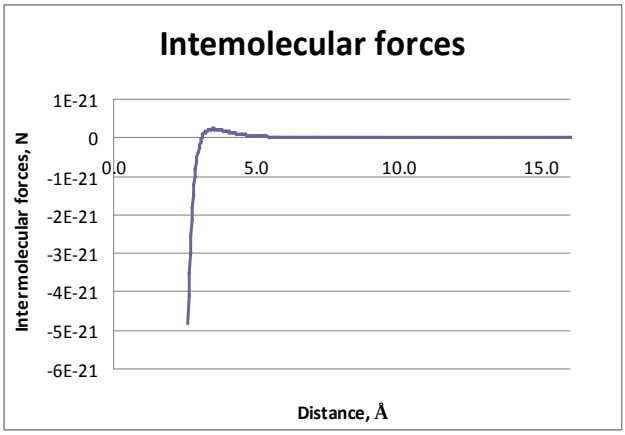

Fig. 2. Intermolecular forces

Simulation model

To ease modeling and visualization we start with some simplifications. All of the simulated molecules have same propitiates. In the case of the actual fluid of the human body there are many other chemical elements. However their number is much (about two orders of magnitude) smaller than those of the water and we will ignore them.

In order to make numerical simulation we need to have estimation of the values ε and σ.

It is known that Avogadro number (number of particles in 1 mol) is 6.022e23.

The mass of one Hidrogen atom is

$$m_H = 1{,}00794\, g/mol = 1{,}67 \cdot 10^{-27}\,\text{kg}. \quad (3)$$

The mass of the Oxigen atom is

$$m_O = 15{,}9994\, g/mol = 2{,}66 \cdot 10^{-26}\,\text{kg}. \quad (4)$$

Thus the mass of one molecule of water (H_2O) is $m_{H_2O} = 2{,}99 \cdot 10^{-26}\,\text{kg}$.

Density of the water at 20° is $\rho = 998{,}2\, kg/m^3$.

So number of water molecules in 1 m^3 is

$$N_{3D} = \frac{998{,}2\, kg/m^3}{2{,}99 \cdot 10^{-26}\,\text{kg}} = 3{,}34 \cdot 10^{28}/m^3 \quad (5)$$

Then number of molecules is a linear meter should be

$$N_{1D} = \sqrt[3]{3{,}34 \cdot 10^{28}/m^3} = 3{,}22 \cdot 10^{9}/m. \quad (6)$$

Finally average distance between water molecules is

$$r_0 = \frac{1}{3{,}22 \cdot 10^{9}/m} = 3{,}11 \cdot 10^{-10}\, m. \quad (7)$$

In order to calculate distance at which inter-particular potential is zero σ, we can use average distance we just calculated r substituting them in (2), when (2) is equal to zero

$$4\varepsilon\sigma^6\left(-12\sigma^6 r^{-13} + 6r^{-7}\right) = 0, \quad (8)$$

or even simpler:

$$-12\sigma^6 r^{-13} + 6r^{-7} = 0. \quad (9)$$

After substitutions we get

$$\sigma = \sqrt[6]{\tfrac{1}{2} r^6} = \sqrt[6]{\tfrac{1}{2} 3{,}11 \cdot 10^{-10}\, m^6} = 2{,}77 \cdot 10^{-10}\, m. \quad (10)$$

For rough estimation of the depth of the potential well ε we will consider thermal kinetic energy as it is given in [3]

$$E_k = \frac{3}{2} kT, \quad (11)$$

where T – temperature measured in Kelvins; k – the Boltzmann constant $1{,}3806504 \cdot 10^{-23}\, J/K$.

From the classical physics is known that kinetic energy is

$$E_k = \frac{mv^2}{2}. \quad (12)$$

Substituting (5) in (6) and solving for v we get average speed of a single particle

$$v = \sqrt{\frac{3kT}{m}}. \quad (13)$$

This gives us some estimated average speed of a molecule at 300K of 645 m/s. This will be used to set initial conditions of our system.

On the other hand calculating kinetic energy from (5) at temperature of $100^{\circ}C$ or 373K (boiling point of water) gives us an estimation for ε, the depth of the potential well since that it would be a temperature at which those intermolecular forces are overcome. It is calculated to be $7{,}72 \cdot 10^{-21} J$ in those conditions.

For easier visual presentation the model we use is done in 2-dimensional space. Thus we will be able to perceive qualitative characteristics of the process without precise quantitive requirements from the results of the simulations.

Algorithmic implementation

Algorithm of the simulation if linear and consists of execution in an infinite loop of the following steps:

1. Initial setup of the particle properties like position and initial speed which is randomly distributed.
2. Visualizing current state of the system.
3. For each particle calculate new state from the current one and the intermolecular influences.
4. Check for the user interaction and go back to step 2.

Most of the processing concerning simulation is done in the step 3. It can be split into following sub steps:

a. Pick next (or first) particle for processing.
b. Compute intermolecular force between current particle and all other with formula (2). Add all those forces together into resultant force $\vec{F}_R$.
c. Compute acceleration that will be created by that force:

$$\vec{a} = \vec{F}_R / m. \quad (14)$$

d. Compute the new speed of the particle from its old speed and the current acceleration:

$$\vec{v} = \vec{v}_0 + \vec{a} \cdot dt. \quad (15)$$

e. Compute the new position of the particle from its old position and its new speed:

$$\vec{x} = \vec{x}_o + \vec{v} \cdot dt. \quad (16)$$

f. If this is not the last particle, go back to step a.

Simulation results

As initial configuration of the molecules we use 2D grid with all the particles forming squares among themselves. To all of them will assign some random initial speed v_0 in the range of the values calculated by (7). It is worthy to note that the actual speed of the molecules is smaller than the given above. Reason for this is that part of thermal energy is manifested in rotation and vibration of the water molecules themselves. As stated earlier the mentioned calculation (7) will be used as a rough estimate of the actual speed.

The initial configuration of our simulation is given in the Fig. 3.

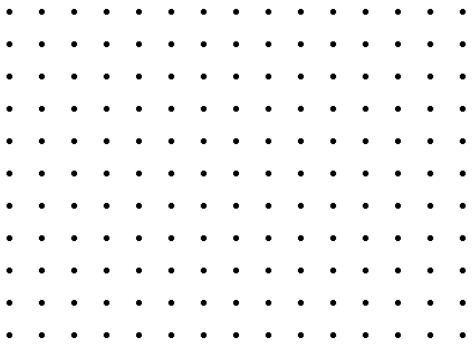

Fig. 3. Initial configuration of the simulation.

This initial configuration very fast is changed as shown on the Fig. 4.

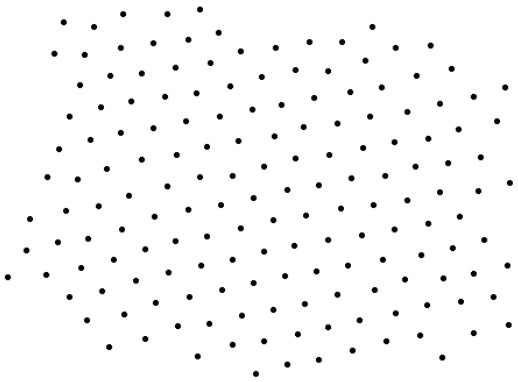

Fig. 4. Configuration of the particles after some simulation steps.

It is visible that all the particles are clustered as it would be natural for a liquid state. Moreover, baring some of the edge particles, it dissembles a close packaging in a 2D space, requiring lower energy. This effect was not engineered but came as a result of the mere application of the formula (1). Thus, it gave initial credibility to the proposed model.

Next experiment is to observe development of the total energy of the system. The simulation recorded value of the total kinetic energy for each step of the algorithm. The chart is given at the Fig. 5.

It is visible that the kinetic energy at first starts low but then increases around certain value and afterwards fluctuates around it. It can be explained by the fact that initial configuration is not in stable state, but having larger amount of potential energy, part of which is later transformed into kinetic energy. Somewhere around step 100 of the simulation, dynamic equilibrium is achieved. After that point approximate levels of both energies are stable further on.

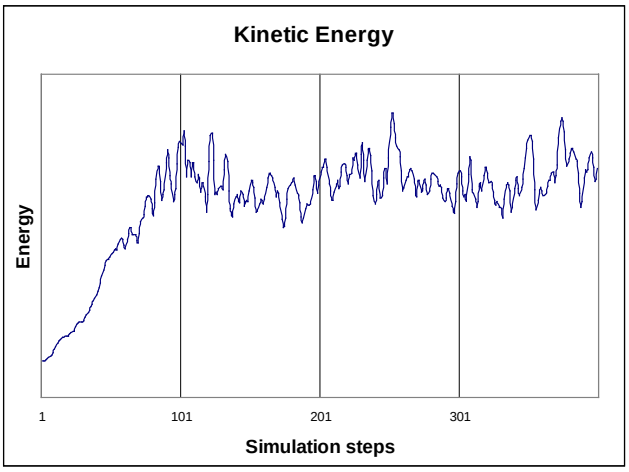

Fig. 5. Kinetic energy of the system

This is another effect coming directly from the model which confirms the stability of the algorithm and its correctness.

Further directions

Additional speedup of the algorithm for bigger sets of data can be achieved with additional data structures and optimized search of the relevant neighboring particles and ignoring those whose influence is so small that it can be neglected.

Additional properties of the model can be added in order to make simulation closer to reality. This includes more precise physical model and execution of the whole simulation in 3D space.

Conclusions

The proposed model for simulation of the physical world reassembles very closely some of the main characteristics of the modeled system.

The achieved results are visually plausible and a give qualitative representation of the system behavior.

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2. **Clark J.** Intermolecular Bonding – Van der Waals Forces, 2000. http://www.chemguide.co.uk/atoms/bonding/vdw.html.

3. **Nave R.** Average Molecular Kinetic Energy. http://hyper physics.phy-astr.gsu.edu/Hbase/kinetic/molke.html

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D. Dimitrov, Z. Cvetkov, S. Guergov. Simulating Fluid Dynamics of the Alive Tissues with Brownian Motion // Electronics and Electrical Engineering. – Kaunas: Technologija, 2010. – No. 4(100). – P. 113–116.

An effort is made to model movement dynamics of atoms and molecules in a fluid of the human body. Thermodynamical and electromagnetic properties of the particles are of main interest. In the current study those are considered to determine their movement features. Ill. 5, bibl. 3 (in English; abstracts in English, Russian and Lithuanian).

Д. Димитров, З. Цветков, С. Гергов. Моделирование динамики флуидов живых тканей броуновским движением // Электроника и электротехника. – Каунас: Технология, 2010. – № 4(100). – С. 113–116.

В статье сделана попытка создать компьютерную модель движения атомов и молекул в жидкости ткани человека. Большой интерес представляют термодинамические и электромагнитные свойства атомов и молекул в жидкости ткани человека. Исследование проводилось имея ввиду эти свойства атомов и молекул в жидкости ткани человека. Ил. 5, библ. 3 (на английском языке; рефераты на английском, русском и литовском яз.).

D. Dimitrov, Z. Cvetkov, S. Guergov. Skysčių dinamikos gyvuose audiniuose modeliavimas įvertinant Brauno judėjimą // Elektronika ir elektrotechnika. – Kaunas: Technologija, 2010. – Nr. 4(100). – P. 113–116.

Aprašytas bandymas sukurti kompiuterinį atomų ir molekulių judėjimo žmogaus audinių skysčiuose modelį. Daug dėmesio skiriama dalelių termodinaminėms ir elektromagnetinėms savybėms, kurios ateityje leis nustatyti dalelių judėjimo būdą. Il. 5, bibl. 3 (anglų kalba; santraukos anglų, rusų ir lietuvių k.).

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