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MOLECULAR HYDRODYNAMICS OF TSUNAMI WAVES

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Abstract. We have developed a molecular dynamic approach for studying tsunami generation. In a two-dimensional model developed a force, which models the generation of disturbance, was incorporated into the water after reaching thermodynamic equilibrium. The temporal evolution of an arising wave shows that at first the disturbance creates the wave of large amplitude which propagates with a significant velocity and a cavity at the site of disturbance. When the wave reaches shallow water, the amplitude and velocity decreases, and the wave changes its shape that is consistent with observations for areas with a large angle of bank. As the bank is approached, the wave density decreases, and foam formation takes place. From the very beginning the surface layer has a lesser density, as if one has "rarefied" water. During the wave propagation the rarefied water penetrates deeper.

1. Introduction

The last quarter century increasingly began to study and investigate the problem of tsunami waves. Tsunami waves ranked the fifth most dangerous natural disaster. People live in cities that are situated on the coasts of oceans and seas, so the question of the study of tsunami waves has great importance. The last major earthquake in January 2004 in the Indian Ocean demonstrated the importance of studying this natural phenomenon when were killed more than 235,000 people and over a million left homeless. This tsunami was recognized as the most devastating natural disaster of the century.

The problem of simulation of tsunami waves is associated with the most diverse forms of generation, distribution and release of the tsunami waves on the shore. In this work, we have applied the molecular dynamics approach to the problem of the landfall of tsunami waves. To simulate this task, it was necessary to write a program that would be implemented by the molecular dynamics method applied to the problem under consideration. Molecular dynamics method avoids many problems associated with traditional styling, but in its turn there are difficulties, for example water as a study material is very complex and not fully understood. When simulating water, there is a shortage of computing power due to complex interactions between atoms of different molecules and the intermolecular interaction between the atoms. In this work numerical investigations were done in such a way that the water molecule was replaced by a single particle which has interacted with other particles. In order to simulate a large number of particles within the available computing time, we have taken a two-dimensional model for studying the output of waves on shore [1-3].

2. Theoretical foundations

Molecular dynamics. The equations of motion used in molecular dynamics are:

$$m_i \frac{d^2 \mathbf{r}_i}{d t^2} = \mathbf{F}_i + m_i \mathbf{G} = \sum_{j=1,\, j \neq i}^{N} \mathbf{F}_{ij} + m_i \mathbf{G} .$$

Here t is the time, $\mathbf{r}_i$ is the radius-vector of particle i, m_i is its mass. The force $\mathbf{F}_i$ acting on a particle is the sum of interaction forces between particles and the gravity force $m_i \mathbf{G}$, which serves as a natural condition due to the particles occupy the allocated space and form a free surface. To describe the interaction of particles we used the Lennard-Jones potential 6-12, which canonical form can be written as

$$U(R) = 4\varepsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^{6} \right].$$

Here the parameter ε gives the depth of the potential well, the parameter σ defines the radius of repulsion and can be found from the condition $U(\sigma) = 0$. To reduce the computational operations, a cutoff radius of the potential was introduced.

There are various numerical schemes for solving the classical equations of motion, from the simplest first order Euler's methods to the predictor – corrector scheme of high order accuracy. We have used the Verlet method in the velocity form as an approach to the time discretization of motion equations because of its simplicity with sufficient accuracy [4].

Boundary conditions. The boundary condition for an opposite coast was chosen as a rigid wall as well as the boundary condition for an oblique relief coast (Fig. 1). The top edge of water was set free, and this is one of the advantages of modeling by molecular dynamics, as the communication area with water and without it is done automatically, without any equations to describe the process. The computational domain is shown in Fig. 2. The calculations were carried out according to the parameters taken from literature [2-4], the system consisting of 6,431 particles.

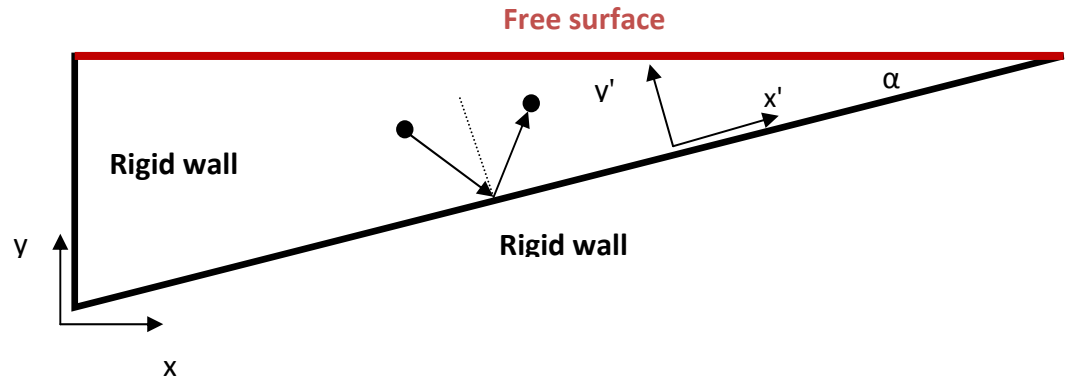

Fig. 1. Computational domain with a particle reflected from the oblique wall.

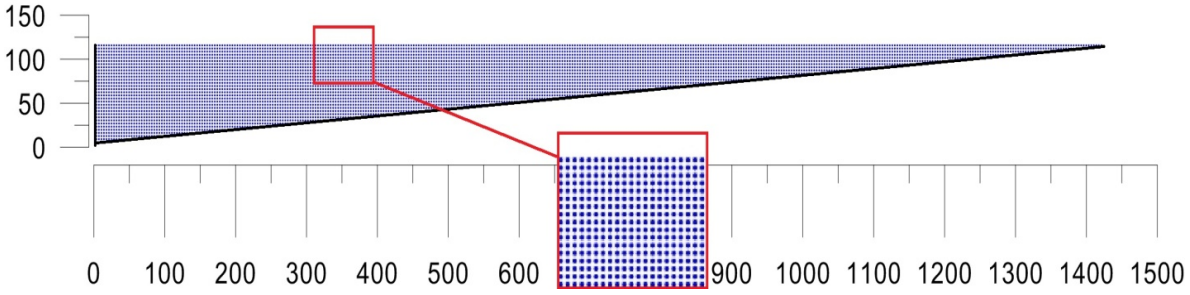

Fig. 2. Overall view of the computational domain with particles at zero time.

Thermodynamic equilibrium. Before starting the wave it is necessary to bring the system in the state of thermodynamic equilibrium at a given temperature. Establishing thermodynamic equilibrium is shown in Figs. 3 and 4.

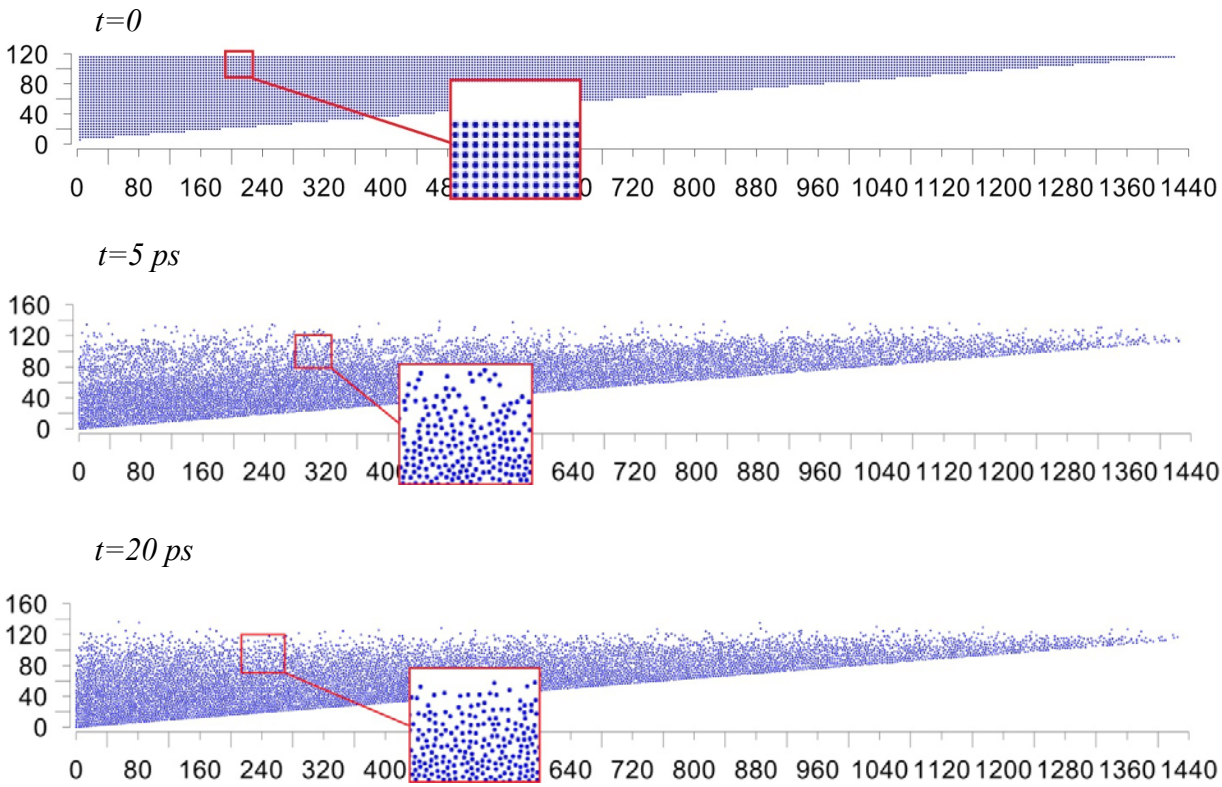

Fig. 3. Evolution of the system to thermodynamic equilibrium;
coordinates are given in Angstroem units.

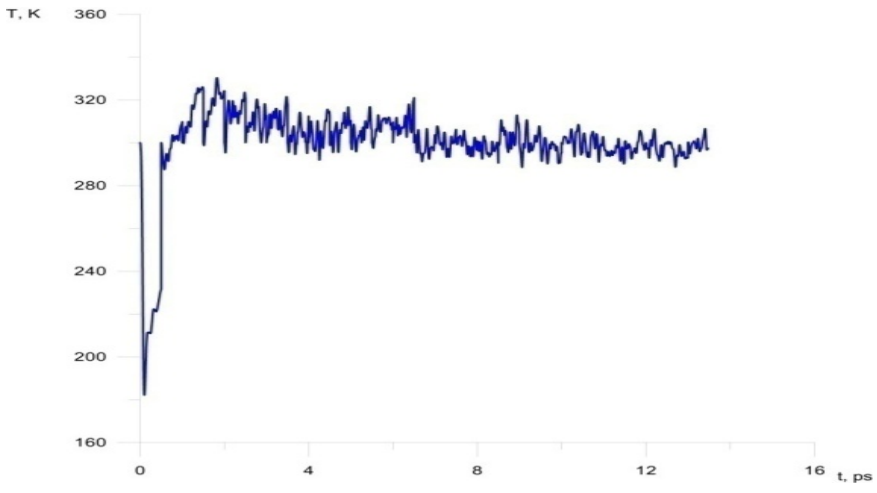

Fig. 4. Temperature dependence on time.

3. Wave generation and propagation

Molecular dynamics allows one to specify any method of wave's initiation by the same equations [5-7]. To obtain the wave we applied a force to the layer of particles located at some distance from the left border (Fig. 5). The force, which models the generation of

disturbance, was incorporated into the water after reaching the thermal equilibrium. The temporal evolution of an arising wave is demonstrated in Fig. 6.

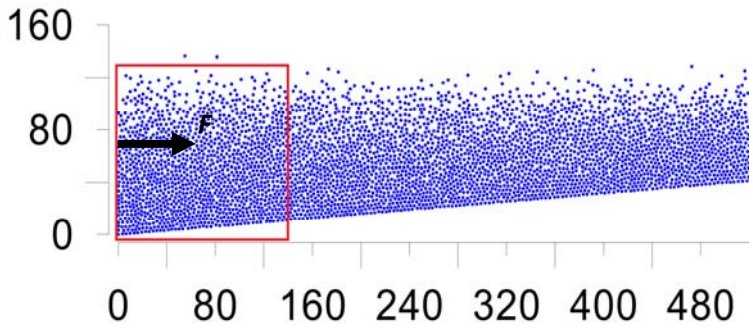

Fig. 5. Region of the particles to which force F was applied.

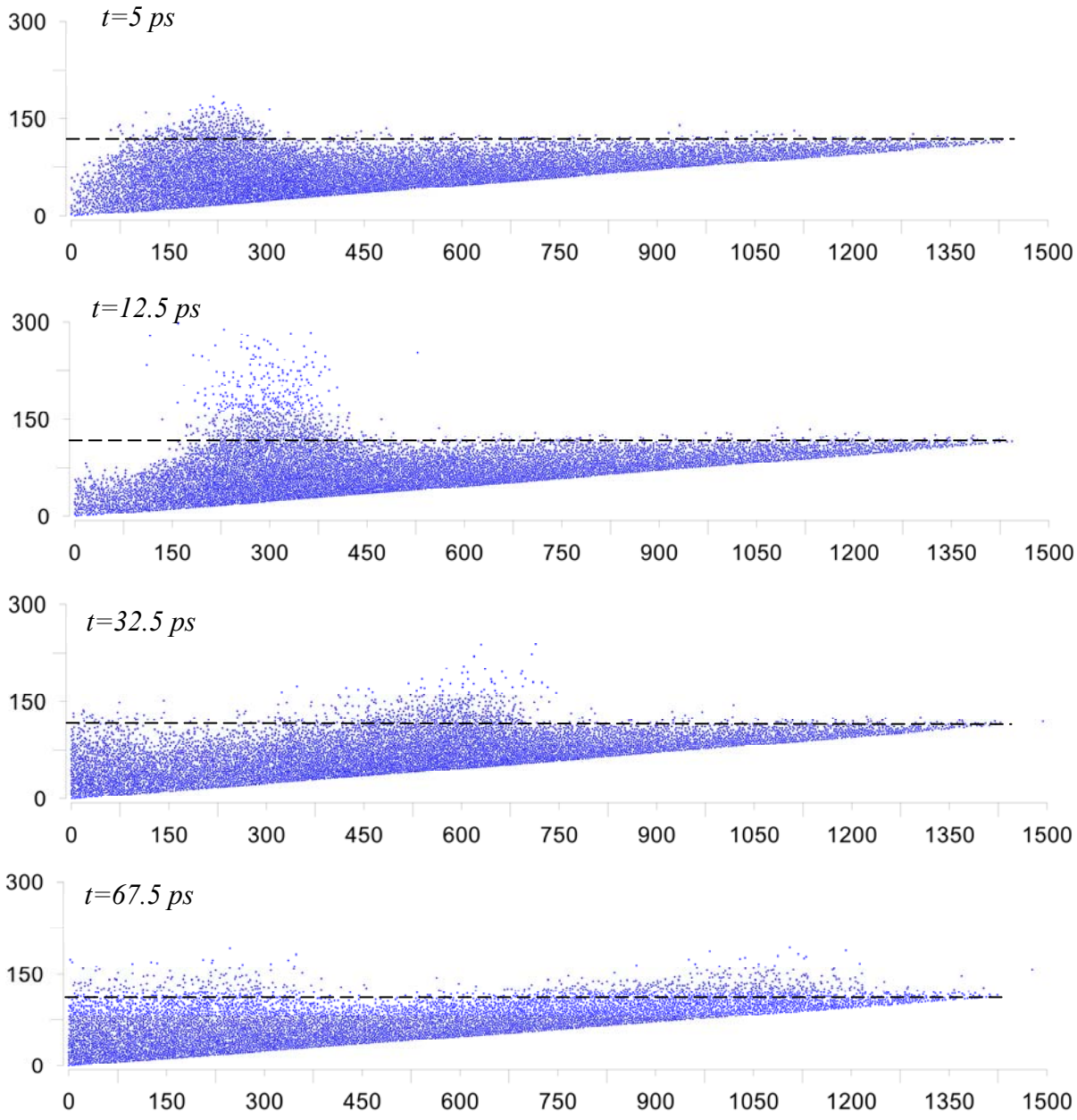

Fig. 6. Wave propagation; coordinates are given in Angstroem units.

At first the disturbance creates the wave of large amplitude which propagates with a significant velocity and a cavity at the site of disturbance (t=5–12.5 ps). When the wave reaches shallow water, the amplitude and velocity decreases, and the wave changes its shape (t=32.5–67.5 ps). This is consistent with observations for areas with a large angle of bank [1, 2].

It is worth noting that as the bank is approached, the wave density decreases, and foam formation takes place. Another interesting detail consists in the following. From the very beginning the surface layer has a lesser density, as if one has "rarefied" water (Fig. 3, t=20 ps and Fig. 5). During the wave propagation the rarefied water penetrates deeper (Fig. 6).

4. Conclusion

We have developed a molecular dynamic approach for studying tsunami generation. Contrary to the customary approach based on different equations of hydrodynamics, which in their turn are based on some postulates, molecular dynamics has evident advantages. Firstly, molecular dynamics is based in fact on the 'first principles' because it uses only two fundamental laws: the second Newton's law of and the Coulomb law. All the potentials of interatomic, intermolecular, interparticle and so on interactions are deduced in reality from the Coulomb law. Secondly, molecular dynamics is an integral method of investigation; it plays the role of a synthesizer of all initial fundamental events, which were incorporated into the model of a process studied. Thirdly, molecular dynamics allows obtain an exhaustive account of all the interactions of the initial fundamental events; in doing so, molecular dynamics operates very prudently without disturbing the liaisons existing in a system. Thus, this method is able to gain a better insight into the nature of tsunami waves.

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