SECTION 3 – MOLECULAR DYNAMICS AND DFT SIMULATION

STRUCTURE OF SHOCK WAVES IN UNDERWATER EXPLOSION

S. Igolkin, A. Melker
Department of Mechanics and Control Processes
St. Petersburg State Polytechnic University, Russia

I. INTRODUCTION. HYDRODYNAMICS, MOLECULAR DYNAMICS, AND UNDERWATER EXPLOSIONS

Until the present time the study of underwater explosions was a privilege of hydrodynamics, which studies the motion of liquids and their interaction with solids. In theoretical hydrodynamics, for description of the movement of an incompressible liquid, having continuity and fluidity, as well as viscosity, one uses the continuity equation and Navier-Stokes' equations. It is difficult to solve this problem by simply writing a complete system of conservation laws in the form of differential equations and closing defining relations, or by developing unique computer programs and codes [1].

Contrary to the customary approach, we have used molecular dynamics [2] for studying underwater explosions. The main motive is such: since the accepted methods of studying "a wealth of phenomena which nature is not well understood" seem to be ineffective, it is reasonable to try other methods. It should be noted that molecular dynamics has shown its effectiveness in studies of a great variety of phenomena, e.g. radiation damage of solids, deformation and fracture of materials, nucleation, evolution and self-organization of biological structures and so on [2]. The problem of modeling underwater explosion, formation and propagation of explosion-generated water waves using molecular dynamics was carefully argued in [3]. In this contribution we used the approach described in that article.

II. COMPUTATIONAL PROCEDURE

We restricted ourselves to 2D computer simulations. To gain a more penetrating insight into the explosion phenomenon, we excluded explosive debris from further research. For this purpose, we developed a simpler explosive model [3]. A certain number of water particles were placed in a circular area of a given size at a predetermined distance. Thereafter the particles were subjected to radial compression. As a result of changing the distance between particles, the compressed structure accumulates a large amount of elastic energy. During decompression these particles acquire enormous velocities, producing an explosion.

In classical molecular dynamics [2], the motion of a system of N particles is described with the help of Newton equations. 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. One of the most common and, at the same time, stable and efficient approach to the time discretization of Newton's equations is the Velocity–Verlet algorithm [4] which was used in the present study as a compromise between speed and accuracy. Integration of the motion equations allows us to find the trajectories of particles. If the initial positions and velocities of the particles are given, the evolution of the system in time depends only on the potential, which determines the interaction between the particles. There are a lot of potentials which are used in molecular dynamics calculations [5]. We have chosen the Lennard–Jones potential. The reasons are given in [3].

III. RESULTS AND DISCUSSION

Movie. The calculations were done with a system consisting of 27,500 particles. An explosive was inserted into the water after reaching the equilibrium. The temporal evolution of underwater

explosion is demonstrated in Fig. 1. Fig. 1a (left) shows the system before explosion; the zoom area specifies the location and structure of explosive. Decompression of the explosive creates a shock wave and a cavity (Fig. 1b, left). It should be emphasized that the cavity is not empty and resembles fog (rarefied water). The expanding shock wave produces a dense compression shock in a narrow region (Fig. 1c, left). Simultaneously, at this moment the shock-wave front reaches the free surface. Thereafter the cavity reaches the surface transforming into a water crater (Fig. 1a, right). The following picture resembles a volcanic eruption (Figs. 1b, 1c, right). At first the volcano is very active and then becomes extinct.

Structure of a shock wave. Up to now there is no complete physical theory describing quantitatively nucleation, development and damping of shock waves. The existing theories, as was mentioned above, have a formal thermodynamical character. The only exception is the book [6] but it contains too many assumptions and became out of date. However, if one wants not only to describe the properties, but understand their nature, one should establish their origin turning to the particles which constituent the system [7]. Unfortunately there is no experimental methods which are able to give such information.

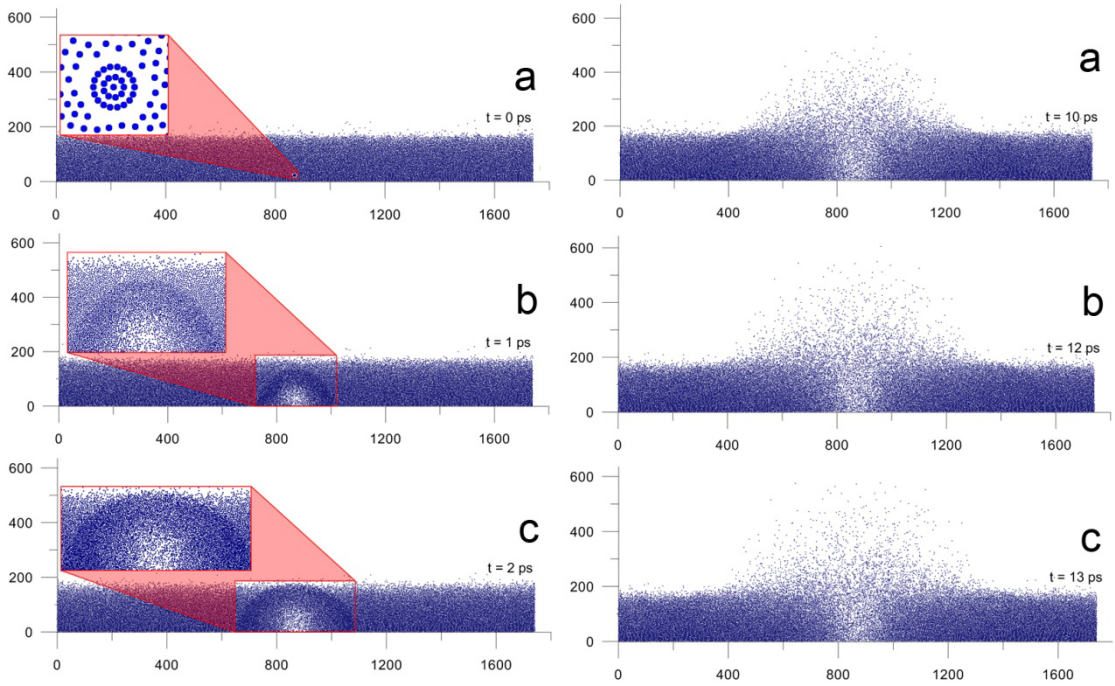

Figure 1 – Time evolution of underwater explosion, t = 0 – 13 ps. Units are in nm-1.

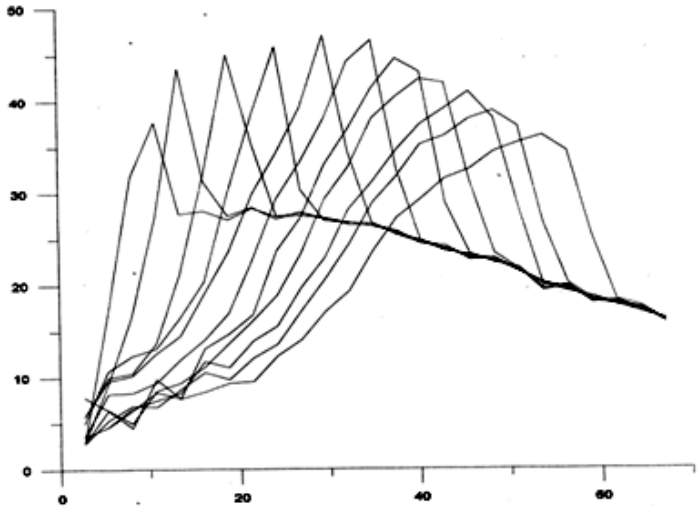

Figure 2 – Time evolution of shock-wave shape, t = 0–5 ps. Units are in nm^{-1}.

In the previous paper [3], we have promised to do the next step, namely, to use one more advantage of molecular dynamics, i.e. to study simultaneously both dynamical structure of a system, observing the motion of separated particle, and to calculate averaged characteristics of the system, e.g. energy, pressure, temperature, etc., especially their distribution in the system and their changing in time. For this purpose we have developed a special technique. The example of such calculation is represented in Fig. 2 which shows the evolution of shock-wave shape in the thirty degree sector (counter-clockwise from x-axis) in an orderly sequence. The wave is moving from left to right.

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