MOVING WINDOW METHOD FOR MODELING STATIONARY SHOCK WAVE IN DIFFERENT MATRERIALS

S. A. Murzov[1, 2], S. A. Dyachkov[1, 2], G. V. Vyskvarko[1, 3], I. S. Galtsov[1, 2, 3], P. R. Levashov[1, 3]

[1]Joint Institue for high temperature RAS, Moscow, Russia

[2]FSUE «Dukhov automatics research institute», Moscow, Russia

[3]MIPT, Moscow, Russia

In numerical simulation of hydrodynamic processes associated with the movement of the object of interest over a considerable distance, often the processes in a limited region of space surrounding the phenomenon or object under study are of interest. Then simulation of the whole computational domain at each moment of time is computationally laborious. For physical reasons, we neglect the influence of distant areas of the computational domain that are insignificant for the phenomenon under study. Instead, a boundary condition can be introduced on the sides of a rectangular region of much smaller size containing the phenomenon under study. The algorithm was first applied with the molecular dynamics simulation [1]. It is aimed at solving the problem of the stress relaxation zone behind the shock wave front takes a considerable time, while simulation facilities are of large cost.

This paper presents a new approach to simulating stationary shock waves in compressible smoothed particle hydrodynamics (SPH) and molecular dynamics (MD) using the developed method of adaptive moving window. The basic idea of the method is that the velocity of this system is adjusted by an iterative feedback algorithm in order to establish the desired position of the shock front. The iterative adaptive moving window algorithm successively estimates the velocity of the shock wave and applies velocity transformations of the reference system to stop the movement of the wave front inside the simulated one. The method has shown faster convergence and applicability for relatively weak shock waves of a mesomechanical porous copper mesomechanical SPH simulation, in contrast to the previously developed moving window algorithm as shown in [2]. In this paper, the method is refined for MD simulation using the example of shock wave calculation in argon. As a result, the shock Hugoniot is obtained, which agrees well with the one obtained in the calculation of the family of isotherms of a small system of atoms and the search for the zero of the Hugoniot function. This work was supported by the Russian Science Foundation under grant No. 24-19-00746.

References

1. **Zhakhovskii, V. V.** Shock wave structure in Lennard-Jones crystal via molecular dynamics [Text] / V. V. Zhakhovskii, S. V. Zybin, K. Nishiohara, S. I. Anisimov // Phys. Rev. Lett. – 1999. – Vol. 83. – P. 1175–1178.

2. **Murzov, S. A.** Adaptive moving window technique for SPH simulation of stationary shock waves [Text] / S. A. Murzov, S. A. Dyachkov, V. V. Zhakhovsky // Comp. Phys. Comm. – 2024. — Vol. 298. – P. 1–16. doi: 10.1016/j.cpc.2024.109116.