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Modeling and Simulation of Shock Wave Propagation at Nanoscale

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ABSTRACT: *Shock wave propagations along a one-dimensional molecule chain were studied in this paper via molecular dynamics modeling and simulation. When the molecule chain is subject to an impact force, oscillations were observed behind the shock wave fronts based on the molecular dynamics simulation results. Such oscillations were mainly due to the numerical errors occurring at strong discontinuities. In this paper, the flux-corrected transport algorithm was implemented in molecular dynamics to overcome this issue. The simulations showed that the proposed method can eliminate the oscillations while keeping the strong discontinuities at the shock wave fronts.*
Keywords: *flux-corrected transport, molecular dynamics, potential, shock wave*

I. INTRODUCTION

Shock waves, like other waves, carry energy and propagate through a medium. The propagation is governed by a second order differential equation, which is hyperbolic in nature, and therefore the shock wave propagation occurs with a finite speed[1]. They are characterized by a nearly discontinuous change in characteristics of the medium, with an extremely rapid rise in pressure, temperature, and density across the shock front. This rapid change can cause deformation, fracture and fragmentation, polymorphic phase changes, and other alterations which can cause failure to occur in materials [2]. Researchers are interested in studying the potentially destructive effects of shock waves both for applications where it is desired, such as military explosions and ballistic impacts, and resistances, such as supersonic flow and military defense.

Experimental studies can be very costly, both in time and material/facility. Therefore, it is preferred to use numerical simulations, whose only major cost is computation time. The simulation of nanoscale mechanics is of growing interest as the area of nanotechnology expands. Molecular dynamics (MD), as a widely-used numerical method at nanoscale, has been employed to study shock wave propagation at nanoscale. Bringa and co-workers [3] used non-equilibrium molecular dynamics (NEMD) to understand about the behavior of metals during the initial phase. Their large-scale MD simulations of up to 352 million atoms provided a detailed understanding of dislocation flow at high strain rates. Other researchers also used MD simulation to study shock-induced phenomena such as phase transitions [4] and chemistry [5, 6].

Because of the nearly discontinuous nature of shockwaves, oscillations are generated behind the shock fronts, which are numerical errors that develop during the simulation. A common technique to remove these oscillations is applying artificial viscosity to the system [7]. While effective at reducing the oscillations, this method spreads the shock wave fronts over several elements and dissipates the total energy in the system. Alternatively, the flux-corrected transport (FCT) algorithm has been shown to remove oscillations without causing these problems, and a finite element with FCT method for the study of shock wave propagation was proposed by Xiao [8].

In this study, we implemented the FCT algorithm in MD simulation to model shock wave propagation at the nanoscale with the removal of oscillations behind shock wave fronts. The outline of this paper is described as below. After introduction, Section 2 provides the methodologies used in this study. Simulations and results are discussed in Section 3 followed by the conclusion.

II. METHODOLOGY

2.1 Molecular Dynamics

MD is a powerful tool that is used to elucidate many physical phenomena at the nanoscale. It assumes that the motion of the molecules in the system obey the laws of classical mechanics. MD simulations are considered excellent approximations for many materials [9]. In a MD simulation, the system is first initialized by selecting initial positions and velocities for each molecule. Once initialization is done, the forces are calculated for each molecule, and positions and velocities are updated through time integration of Newton's equations of motion, shown in (1).

$$\ddot{u} = \frac{f_{ext} + f_{int}}{m} \tag{1}$$

where u is the displacement, the superposed dots represent material time derivatives, f_{ext} is the externally applied force, f_{int} is the internal force, and m is the particle mass. The internal force is derived from the potential energy function as shown in (2),

$$f_{int} = -\frac{\partial U}{\partial r} \tag{2}$$

where U is the total potential, and r is the position of molecule

During the MD simulation, the accelerations are calculated based on the forces, i.e. (1). The velocities are then determined by integrating accelerations, and positions by integrating velocities. In this paper, the time integrations within the time step of Δt were performed using the velocity Verlet method given below.

$$u(t + \Delta t) = u(t) + \dot{u}(t)\Delta t + \frac{1}{2}\ddot{u}(t)\Delta t^2 \tag{3}$$

$$\ddot{u}(t + \Delta t) = -\frac{1}{m}\left[f_{ext} + f_{int}\left(u(t + \Delta t)\right)\right] \tag{4}$$

$$\dot{u}(t + \Delta t) = \dot{u}(t) + \frac{\Delta t}{2}\left[\ddot{u}(t) + \ddot{u}(t + \Delta t)\right] \tag{5}$$

2.2 Flux-Corrected Transport

The FCT algorithm contains two stages, the transport stage and the antidiffusion stage, where the antidiffusion stage corrects the numerical errors from the transport stage. These two stages allow the FCT algorithm to treat discontinuities without generating oscillations. The FCT algorithm was originally used in one dimensional finite-difference (FD) methods. The general FCT is composed of six steps outlined below in (6) through (11).

The first step is the transport calculation, where the trial values of any function Q are obtained at time step n+1 and spatial step j with (6), where Δt is the time step and ΔX is the spatial increment.

$$\tilde{Q}_j^{n+1} = f(Q_j^n, \Delta t, \Delta X) \tag{6}$$

The second step is shown as (7), the calculation of the diffusive fluxes, where η_1 is the diffusive coefficient.

$$\varphi_j^0 = \eta_1\left(Q_{j+1}^n - Q_j^n\right) \tag{7}$$

The third step is the diffusion step.

$$\bar{Q}_j^{n+1} = \tilde{Q}_j^{n+1} + \varphi_j^0 - \varphi_{j-1}^0 \tag{8}$$

Step four is (9), the calculation of the antidiffusive fluxes, where η_2 is the antidiffusive coefficient.

$$\varphi_j^1 = \eta_2\left(\tilde{Q}_{j+1}^n - \tilde{Q}_j^n\right) \tag{9}$$

Step five is to select the limitation of antidiffusive fluxes, where $S = \text{sign}(\varphi_j^1)$, and $\Delta_{j-1} = \bar{Q}_j^{n+1} - \bar{Q}_{j-1}^{n+1}$.

$$\varphi_j^c = S * \max\left\{0, \min\left[S * \Delta_{j-1}, |\varphi_j^1|, S * \Delta_{j+1}\right]\right\} \tag{10}$$

The final step is the antidiffusion step, shown as (11).

$$Q_j^{n+1} = \bar{Q}_j^{n+1} - \varphi_j^c + \varphi_{j-1}^c \tag{11}$$

While the FCT algorithm has been shown to efficiently eliminate oscillations when used with FD methods, it must be applied to each of the several differential equations that are usually needed for FD. For finite element (FE) methods, the same algorithm can be used by only applying the FCT algorithm to the velocity update [8]. Since each component of velocity is independent, the FCT can be applied to each component separately, provided that a structured mesh is used. This algorithm can be extended to MD simulations.

2.3 MD-FCT

With the implementation of the FCT algorithm, the flowchart for the MD simulation can be written as follows:

a) Initialization and initial conditions: give initial positions to the molecules in equilibrium position.

b) Update displacements and accelerations of molecules via equations (3) and (4) at time based on the atomistic displacements, accelerations and velocities at time .

c) Obtain trial velocities via equation (5), , and then apply FCT to velocities:

i) Calculate diffusive fluxes: $\varphi_i^0 = \eta_1(\dot{u}_i^n$.

ii) Diffusion: $\bar{u}_i^{n+1} = \tilde{u}_i^{n+1} + \varphi$.

iii) Calculate antidiffusive fluxes: $\varphi_i^1 = \eta_2(\tilde{u}_i^n$.

iv) Apply limitation of antidiffusive fluxes:

$$\varphi_i^C = S * \max\{0, \min[S * \Delta_{i-1}, |\varphi_i^1|, S$$,

where $S =$, and $\Delta_{i-1} = \bar{u}_i^{n+}$.

v) Antidiffusion: $\dot{u}_i^{n+1} = \bar{u}_i^{n+1} - \varphi$.

d). Output if simulation is complete; if not, return to (b).

III. SIMULATIONS AND DISCUSSIONS

We first considered shock wave propagation in a one-dimensional linear elastic molecule chain with a length of 20 nm. A simple spring model was used for interaction between two neighboring molecules. The potential function is

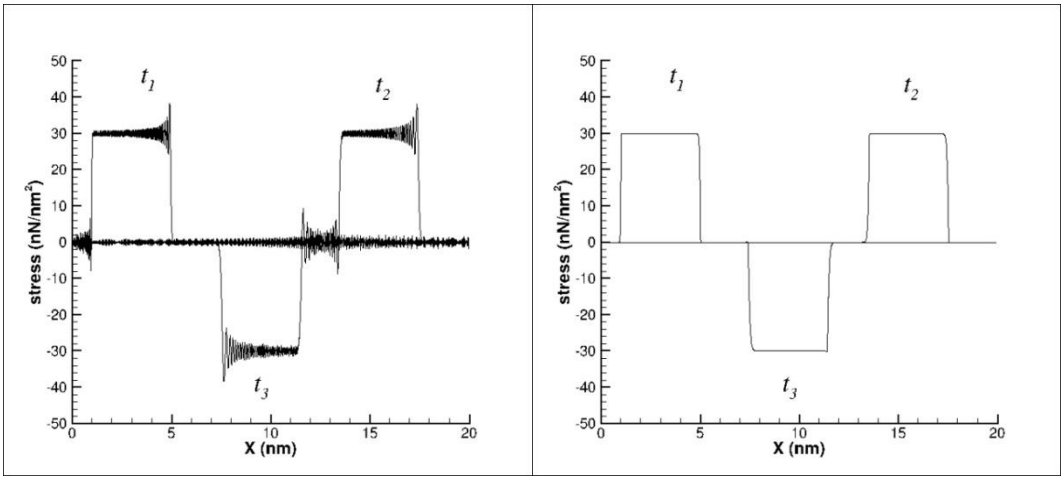
$$U_s = \frac{1}{2}k(r_0 - r)^2 \quad (12)$$

where *k= 100 N/m* is the spring stiffness, $r_0 = 0.01\ nm$ is the unstretched bond length bewteen two neighboring molecules, and r is the current bond length. Each molecule has a mass of 10^{-25} kg. The initial configuration was assumed to be at zero temperature, and molecules were placed at their equilibrium positions. A force with magnitude 30 nN was applied to the molecule chain at one end for 1.3 ps and then released. A free end boundary condition was used for the opposite end of the chain. At nanoscale, the stress is calculated based on the interatomic forces between molecules as the following equation

$$\sigma = \frac{1}{\Omega}\sum_I \left(\frac{1}{2}\sum_{J(\neq I)} r_{IJ} \otimes f_{IJ}\right) \quad (13)$$

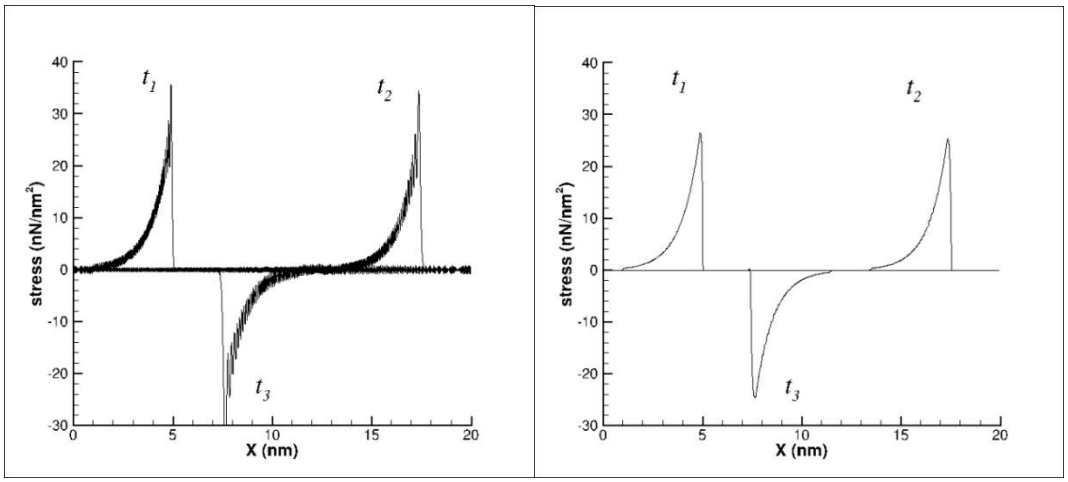
where $r_{IJ}(= r_I - r_J)$ represents interatomic distance between atoms *J* and *I*, and $\otimes$ denotes the tensor product of two vectors. The sign convention adopted here for interatomic forces, f_{IJ}, is positive for attraction and negative for repulsion.

Stress distributions along the molecule chain were plotted at three different times: $t_1 = 1.6, t_2 = 5.5$, and $t_3 = 10.3$ ps as shown in Fig. 1. It can be seen that the oscillations were generated behind the shock fronts during molecular dynamics simulation. After applying the FCT algorithm, a very good discontinuous wave profile can be seen in Fig. 1(b).



(a) MD simulation **(b)** MD-FCT simulation

Fig. 1. square shape stress wave propagating along a one-dimensional molecule chain with a spring-model potential



(a) MD simulation **(b)** MD-FCT simulation

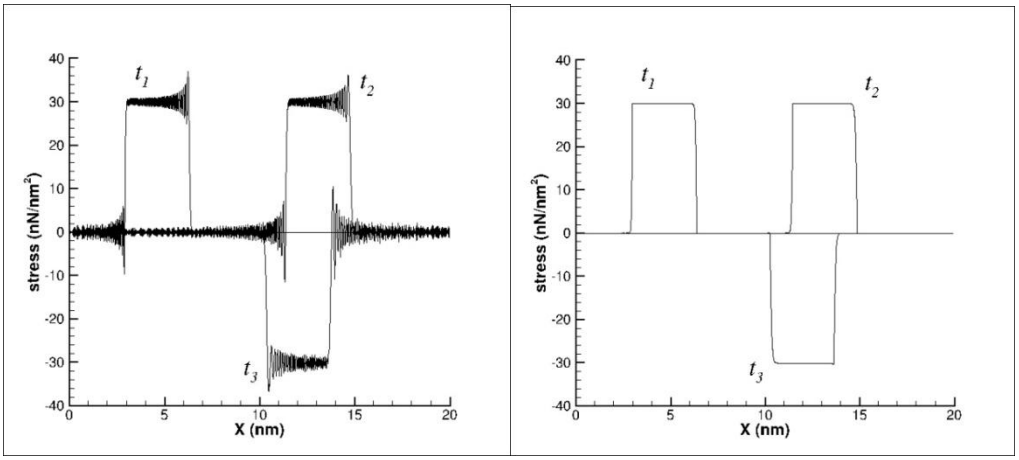
Fig. 2. decaying stress wave propagating along a one-dimensional molecule chain with a spring-model potential

Next, a different wave shape is examined by changing the applied load and keeping all other parameters unchanged. Instead of a constant magnitude, the load exponentially decays after the initial application. Fig. 2 shows the wave with FCT applied and without FCT applied, respectively. It can be seen that the FCT algorithm can remove the oscillations while preserving the discontinuous wave front and the peak of the wave. It should be noted that in both cases the wave perfectly retained its shape as it propagated along the molecule chain. This was due to the spring-model potential being very simple, and its derivative, which was the internal force, being linear. Because the slope for the internal force was constant, it did not matter how high or low the stress was, the stiffness is always the same. Thus, the front (loading) wave and back (unloading) wave always had the same speed, even if the stresses were at different magnitudes.

The second potential function examined is the Lennard-Jones 6-12 (LJ) potential, shown in (14), where $\varepsilon = 10nJ$ is the depth of the energy well.

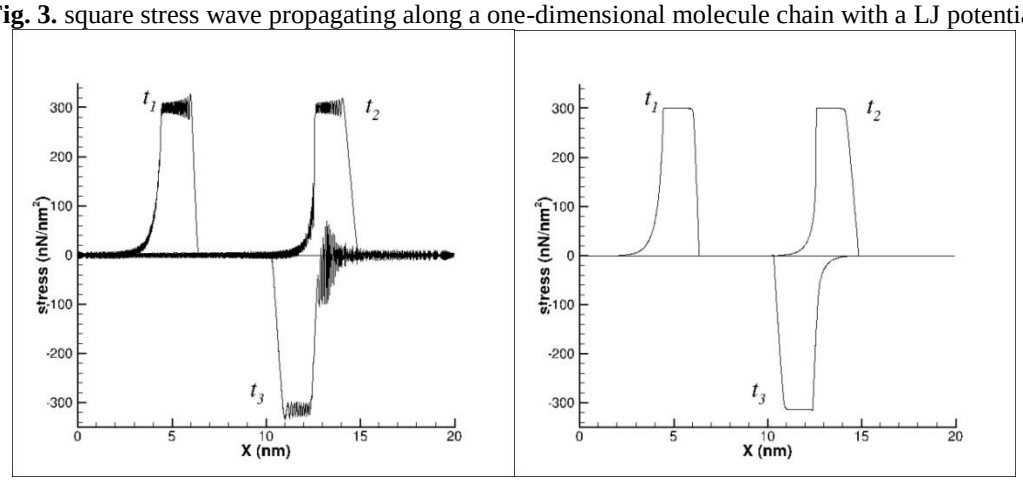
$$U_{LJ} = 4\varepsilon\left[\frac{1}{4}\left(\frac{r_0}{r}\right)^{12} - \frac{1}{2}\left(\frac{r_0}{r}\right)^{6}\right] \tag{14}$$

The same molecule chain was studied as in the above except the LJ potential is employed to describe the interatomic interaction between neighboring molecules. A square stress wave was examined first. A force of 30 nN is applied to the end of the molecule chain for 4.0 ps. The stress waves were plotted at three different times: $t_1 = 7.5$, $t_2 = 17.5$, and $t_3 = 35.0$ ps. Without applying the FCT algorithm, oscillations were again generated behind the shock fronts. Such oscillations can be totally eliminated when implementing the FCT algorithm in MD simulations, as shown in Fig. 3.



(a) MD simulation **(b)** MD-FCT simulation

Fig. 3. square stress wave propagating along a one-dimensional molecule chain with a LJ potential



(a) MD simulation **(b)** MD-FCT simulation

Fig. 4. decaying stress wave propagating along a one-dimensional molecule chain with a LJ potential

It shall be noted that the induced stress was small enough here, and the equivalent stiffness due to the LJ potential was almost a constant. Therefore, the loading and unloading waves had nearly the same (and constant) speed. Consequently, the shape was almost perfectly maintained. However, if the stress was large enough, the equivalent stiffness (second derivative of the potential) was not constant at different stress levels. Therefore, the wave speed at different stress levels would vary. Specifically, higher stresses would cause slower wave speeds. To illustrate such phenomena, a wave similar to the exponentially decaying wave was studied. The initial force magnitude of 300 nN was held for 2.0 ps, and then decayed for 3.0 ps down to zero. The stress waves at three different times were plotted in Fig. 4.

As shown in Fig. 4, the loading wave front sloped back because wave propagated slower at a higher stress level. At unloading phase, since low-stress waves propagated faster than high-stress waves, the unloading wave become more and more abrupt. In addition, the unloading wave caught the loading wave, and the plateau began to shrink.

IV. CONCLUSION

The flux-corrected transported algorithm was implemented in molecular dynamics simulations in this paper to study shock wave propagation at nanoscale. The simulation results showed that the proposed method could easily eliminate the oscillations behind the shock wave fronts as well as maintain the strong discontinuities. Two potential functions were employed, and the shock waves propagated differently. Although only one-dimensional molecule chains were studied in this paper, the proposed method could be easily extended to study multi-dimensional nanosystems. It shall be noted that no temperature effects were considered in this paper because the proposed method could eliminate atomic vibrations as well. Studying the temperature effects on shock wave propagations at the nanoscale could be the future research.

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