Molecular Dynamics Study on Wave Equation of Liquid

Tatiana ZOLOTOUKHINA† and Toshihiro IWAKI†

Abstract

The equation of wave propagating in fluid is described as a differential equation of the velocity or small element density from the Navier-Stokes (NS) equation. On the other hand, the molecular dynamics (MD) equation expresses the motion of a particle constituting the fluid and shows that the particle is always in motion regardless of the existence of the wave. In this study, we discuss in what way meanings of the velocity and density in the wave equation can be adopted in the MD system. What are the differentials with respect to time and space in the NS equation for the system of MD particles? Ordinarily, the physical quantities in the NS equation are obtained as the ensemble and time averages over the MD system. We investigate the number of particles and duration of time that are sufficient for the averages and simultaneously confirm whether the averaged values satisfy the differential equation. The two-dimensional MD method is used for the qualitative understanding. The fluid is assumed to consist of particles connected by the Lennard-Jones potential. The satisfaction of the differential equation by the MD averaged values is shown by the propagation velocity in the wave equation. The propagation velocity can be also obtained in another way i.e. by the 'observation' of the wave fronts motion of velocity, density or total energy wave in the fluid. The propagation velocity that has resulted from the wave equation is strongly affected by the ensemble and time averages. On the other hand, when it is obtained from the wave front, it is independent of the ensemble and time averages. We can have the former propagation velocity close to the latter one when a long time average is used for a large ensemble and a short time average for a small ensemble, i.e. the product of both averages can be considered changed at same rate as if by a scaling coefficient.

Key Words: *Molecular dynamics, Wave equation, Wave front, Liquid*

1 Introduction

Theoretical studies of thermo-fluid phenomena by using the continuum mechanics have been the subject of the ongoing research for several decades because of the extended importance in wide range of practical engineering applications. The continuum characteristics of the thermo-fluid phenomena is obtained by solving governing equations describing conservations of mass, momentum and energy in an extremely small cubic element or unit cell (called thereafter the element) under certain boundary and/or initial conditions. The extremely small cubic element is considered to be homogeneous and continuous there. It is assumed in the continuum mechanics that, in the cubic element, the temporal and spatial deviations of the physical quantities such as density or pressure from their average values are very small. This assumption enables the deviations to be linear. Then we can ignore the terms higher than second order one of the Taylor's series expansion and represent the deviation by the first order derivative. Therefore, the governing equations are expressed by differential equations. This differential equation approach represents the approach to the physical phenomena that are considered continuous. The study using the continuum mechanics is the macroscopic one.

However, from the physical viewpoint, the cubic element consists of many atoms and/or molecules in motion at high velocity. The element is not continuous but discrete microscopically. Atoms and molecules are assumed to be called particles hereafter. The motion of a particle is expressed by the MD equation and then the cubic element is nothing but a limited volume of space. Particles don't (continuously) always stay in a certain cubic space and may move in or out from the cubic space to the neighboring elements due to their individual motion. The cubic element is not homogeneous in relation to the number and type of particles that are moving inside it.

Due to the duality of approaches, here we have a very important and fundamental problem of connection between the continuum mechanics and the particle motion outlined by the following questions. How the physical quantities in the governing equations of the

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continuum mechanics are derived from characteristics of the particle motion? What are definitions of differentials ∂x and ∂t of the governing equations in the MD system? Namely, how can the MD method connect particle motion to the continuum mechanics? The answer to the problem will make clear how small a unit size and how short a time interval can be applied in the continuum mechanics in the limit of small scale.

For the problem stated, the governing equations of the continuum mechanics were derived from the MD equations [1-4] by Kotake. He concluded that the local uniformities in the temporal and spatial scales are necessarily demanded in the MD system for the connection of particle motion to the continuum mechanics. If the MD system has no such local uniformities, it cannot explain even non-equilibrium and/or unsteady state macroscopic mechanical phenomena. These conclusions lead us to discuss what the local uniformities are and then how they are obtained in the real MD simulation.

In order to determine the local uniformity, the plane elastic wave, that is a propagation of disturbed displacement of an extremely small cubic element in an elastic solid continuum, was investigated as one of the typical non-equilibrium and unsteady state macroscopic mechanical phenomena [5]. It was found that, if an appropriate average value of particle displacement with respect to space and time in the MD system was defined as the displacement of a point in the elastic solid continuum, it behaved like in the wave equation of the continuum mechanics.

There are many types of disturbances propagating in a medium besides the displacement wave and are different mediums propagating various types of disturbances. Therefore, it would be important to compare whether some or all features and behavior of chosen disturbances are same as the displacement wave. In the present study, propagations of disturbed velocity and density waves in a liquid are investigated. They are compared with the plane elastic wave. Although, the wave propagation of the energy disturbance is not described by the same type of the wave equation as the motion of the disturbance in velocity or density waves, it is also examined.

We use Lennard-Jones particles and calculate their motions by means of the two-dimensional MD method for understanding of the phenomenon qualitatively.

2 Wave Equation and Particle Motion

In the continuum mechanics, the wave equation for disturbed velocity (or density waves), u, is expressed by

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{1}$$

under the conditions of stationary fluid and an isentropic change, where c is a propagation velocity and is given

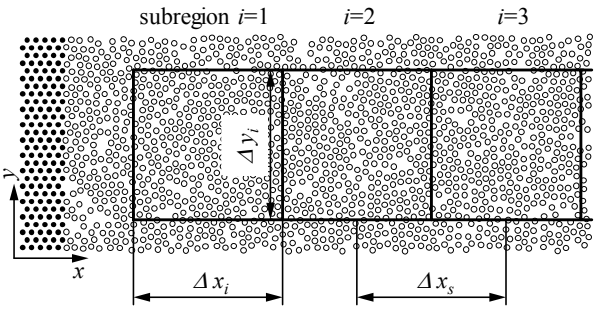

Fig. 1 Particles near the left end of the MD system and definition of subregion.

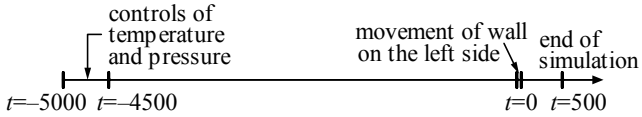

Fig. 2 Time development of calculation procedure.

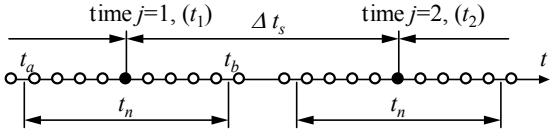

Fig. 3 Average with respect to time and definition of time interval.

by

$$c^2 = \left(\frac{\partial P}{\partial \rho} \right) \tag{2}$$

or

$$c^2 = \gamma \frac{P}{\rho} \tag{3}$$

where P, ρ and γ are pressure, density and specific heat ratio, respectively. There is no wave motion without disturbance, and a region of disturbance propagation should have a coherent change in respective values of the wave. On the other hand, the particle is always in motion regardless of the wave. The motion of a particle constituting the liquid is expressed by the MD equation

$$m \frac{\partial^2 \boldsymbol{x}}{\partial t^2} = \boldsymbol{F} \tag{4}$$

where m and $\boldsymbol{x}$ are the mass and position of the particle, respectively, and $\boldsymbol{F}$ is the force acting on the particle.

3 Model and Calculation Method

The potential of the Lennard-Jones particl is

$$\phi_{\alpha,\beta} = 4\varepsilon \left\{ \left(\frac{\sigma}{r_{\alpha,\beta}} \right)^{12} - \left(\frac{\sigma}{r_{\alpha,\beta}} \right)^{6} \right\} \tag{5}$$

where ε, σ and $r_{\alpha,\beta}$ are the potential depth, the length parameter and the distance between particles α and β, respectively. We have the following dimensionless energy, pressure, length, temperature, time, velocity and density.

$$\frac{1}{24\varepsilon}e \to e,\ \frac{\sigma^f}{24\varepsilon}P \to P,\ \frac{1}{\sigma}r \to r,\ \frac{k_B}{24\varepsilon}T \to T,$$
$$\sqrt{\frac{24\varepsilon}{m\sigma^2}}t \to t,\ \sqrt{\frac{m}{24\varepsilon}}v \to v,\ \frac{\sigma^f}{m}\rho \to \rho \qquad (6)$$

Here k_B and f are Boltzmann's constant and dimension, respectively. We set f=2 for the two-dimensional MD method.

Figure 1 shows a particle configuration close to and at the disturbance generation region on the left end of the MD system. The unfilled circles (○) show liquid particles, their number being 17360. The number of particles of two rigid walls marked by filled circle (●) at the left and right ends is 280. The periodic boundary condition is employed in the y direction. The equation (4) of molecular motion is transformed into the difference equation and the time difference Δt=0.01 is used. Particles are set in motion under the conditions of temperature T=1.95×10^{-2} and pressure P=5.10×10^{-3}. If the particles are argon atoms, the time difference is equal to 4.4 fs and the temperature is 55K. As shown in Fig. 2, we put t=0 after a considerably long time elapses. In order to investigate the direction of the wave, the rigid wall on the left hand side is moved to the distance 0.677 at an angle of 60° relative to the x axis during the time duration of 10.38.

The physical quantities in the continuum mechanics are obtained from the spatial and temporal averages of the properties of MD system. Therefore, the point of matter is focused on how large space region and how long time are required for the wave equation (1). For the spatial average, a series of subregions are defined in the liquid and are named subregion i=1, 2, 3 and so on from the left hand side to the right hand side as shown in Fig. 1. Four kinds of subregion width are employed i.e. Δx_i=20, 40, 80 and 160. We always have Δy_i=20. Then the average numbers of particles $\overline{\langle N_i \rangle}$ are 288, 577, 1153, and 2307, respectively, where N_i is the number of particles in a subregion i, the symbols $\langle\ \rangle$ and $\overline{\ }$ mean the averages with respect to subregion and time, respectively. The distance between the neighboring subregions is denoted by Δx_s and is used as ∂x in the wave equation (1). We set Δx_s=Δx_i. As shown in Fig. 3, the average time between t_a and t_b is expressed as t_n=$n\Delta t$ and four kinds of n =99, 999, 2999, and 9999 are taken. The values averaged with respect to time are defined as those at the middle time j (t_j). The time interval Δt_s between the neighboring average values is set to be equal to $n\Delta t$ and is used as ∂t in the wave equation (1).

We define the disturbed velocity, density, total energy and pressure in a subregion i at a time j as

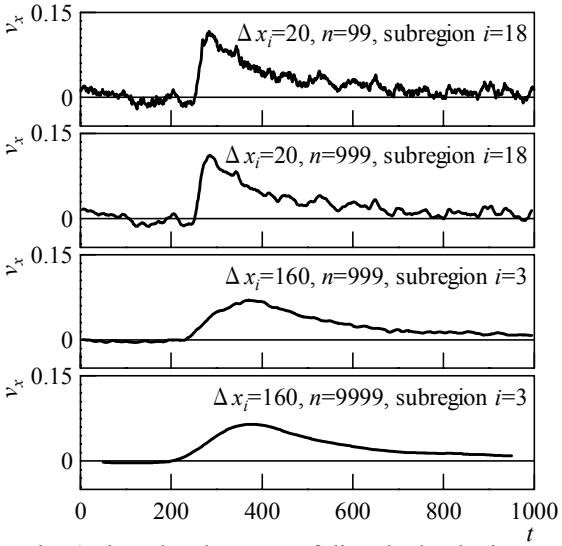

Fig. 4 Time development of disturbed velocity v_x.

$$\boldsymbol{v}_{i,j} = \frac{1}{n}\sum_{k=-(n-1)/2}^{(n-1)/2}\left(\frac{1}{N_i m}\sum_{\alpha=1}^{N_i} m\boldsymbol{v}_\alpha\right)_{t_j+k\Delta t} \qquad (7)$$

$$\rho_{i,j} = \frac{1}{n}\sum_{k=-(n-1)/2}^{(n-1)/2}\left(\frac{N_i}{S_i}\right)_{t_j+k\Delta t} \qquad (8)$$

$$e_{t_{i,j}} = \frac{1}{n}\sum_{k=-(n-1)/2}^{(n-1)/2}\left(\frac{1}{S_i}\sum_{\alpha=1}^{N_i} e_{t_\alpha}\right)_{t_j+k\Delta t} \qquad (9)$$

$$P_{i,j} = \frac{1}{n}\sum_{k=-(n-1)/2}^{(n-1)/2}\left(\frac{1}{S_i}\sum_{\alpha=1}^{N_i} p_\alpha\right)_{t_j+k\Delta t}$$
$$p_\alpha = \frac{1}{f}m_\alpha v_\alpha^2 + \frac{1}{2f}\sum_{\beta=1}^{N_i}\boldsymbol{r}_{\alpha,\beta}\cdot\boldsymbol{F}_{\alpha,\beta} \qquad (10)$$

respectively, where $\boldsymbol{v}_\alpha$ and $e_{t\alpha}$ are the velocity and total energy of particle α, respectively, and S_i is the area of the subregion i. The derivatives at both sides of Eq. (1) are transformed into the difference equations. For example, the left side is

$$\frac{\partial^2 u}{\partial t^2} = \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta t_s)^2} \qquad (11)$$

The macroscopic propagation velocity, c, is calculated from the MD system by use of Eqs. (1) and (11).

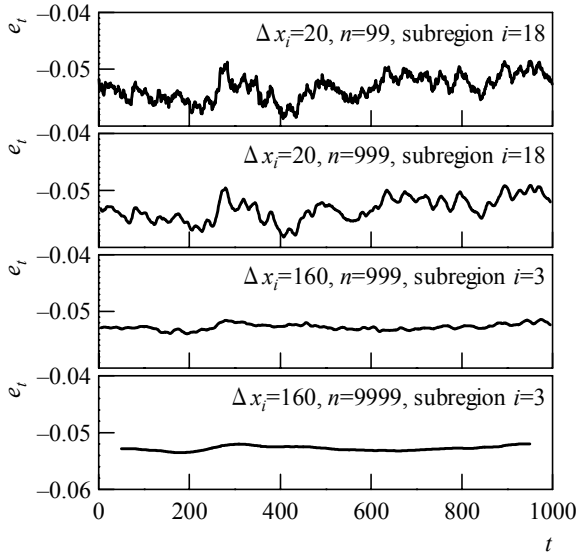

Fig.5 Time development of disturbed total energy e_t.

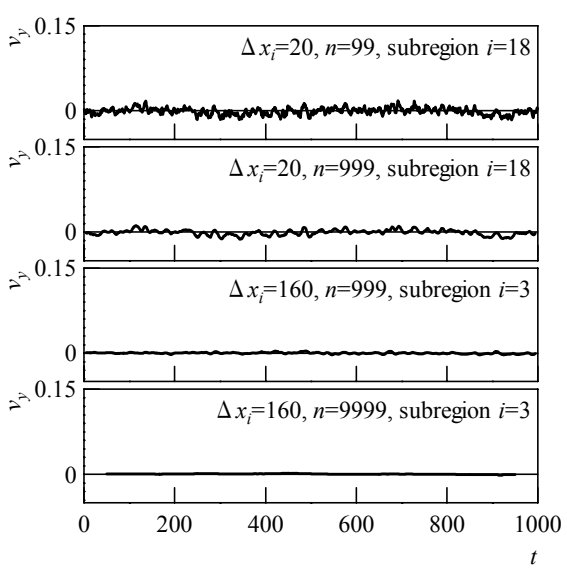

Fig.6 Time development of disturbed velocity v_y.

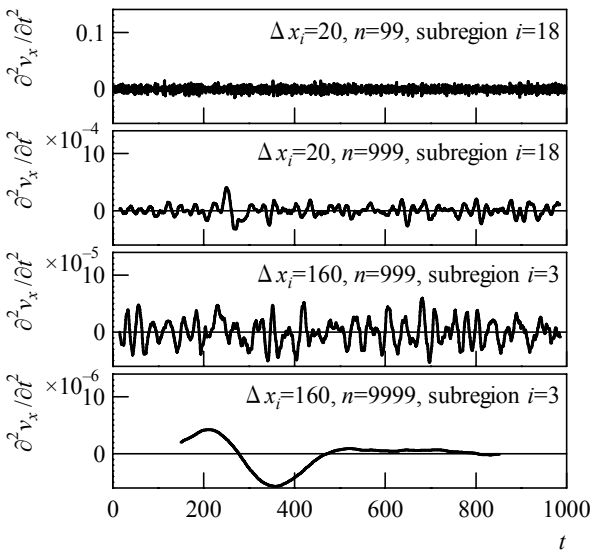

Fig. 7 Time development of $\partial^2 v_x/\partial t^2$.

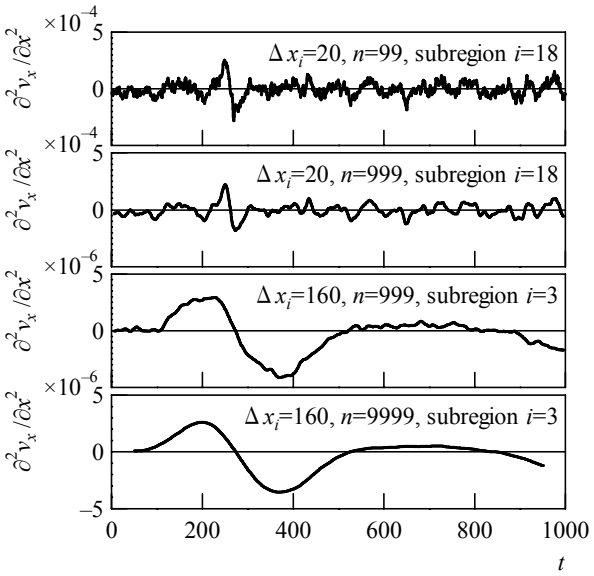

Fig.8 Time development of $\partial^2 v_x/\partial x^2$.

3 Results and Discussions

3.1 Averages with respect to particle and time

Figure 4 shows the time development of disturbed velocity v_x and is arranged from the top to the bottom by amounts of average i.e. (Δx_i=20, n=99), (Δx_i=20, n=999), (Δx_i=160, n=999) and (Δx_i=160, n=9999). As shown in the figure, the disturbed velocity increases abruptly at t≈250 as if an arrival of a wavelike matter because the value of the disturbed velocity is almost zero before the arrival. After then, it decreases gradually and is approaching to zero again. Therefore we can consider that the abrupt increase is the disturbed velocity wave. As shown in the top graph of Fig. 4, the value of the disturbed velocity before the arrival of the wave is not exactly zero and this result is different from one in the continuum mechanics. If the amount of average is large, the disturbed velocity increases gradually as time elapses as shown in the bottom graph of Fig. 4. The value of the disturbed velocity before the arrival of the wave is almost zero as if in the continuum mechanics. The maximum value of v_x decreases and the small fluctuations of high frequency of the curve disappear as the amount of average becomes large. The time of the maximum disturbed velocity comes later for the case of large subregion (Δx_i=160) relative to small subregion (Δx_i=20). It is concluded that the disturbed velocity curve strongly depends on the amount of average with respect to time and space. The features of the disturbed velocity for the other cases of the amount of average are

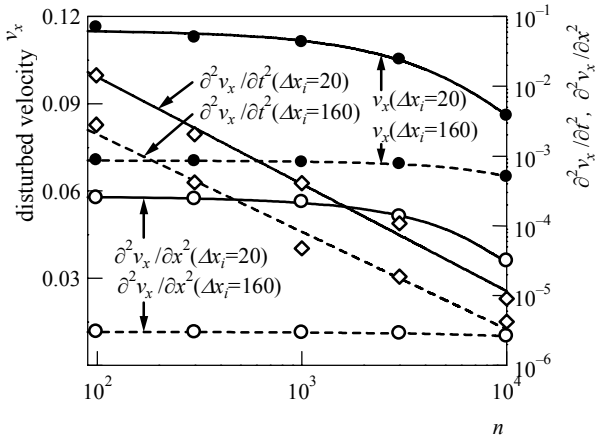

Fig. 9 Maximum values of disturbed velocity v_x and its derivatives $\partial^2 v_x/\partial x^2$ and $\partial^2 v_x/\partial t^2$ vs. number of averages.

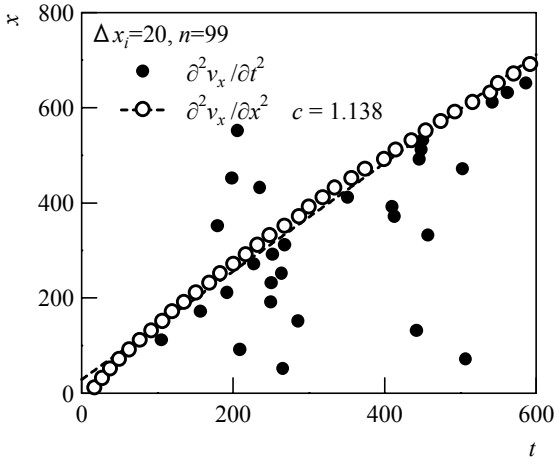

Fig. 10 Position of wave front (for the case of small amount of average) as changed with time.

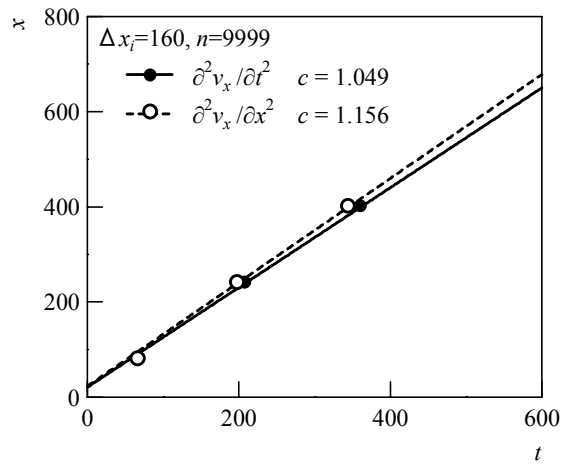

Fig. 11 Position of wave front (for the case of large amount of average) as changed with time.

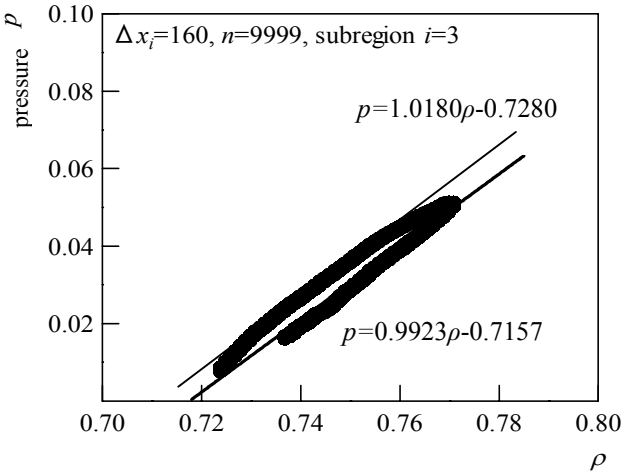

Fig. 12 Relation between density and pressure.

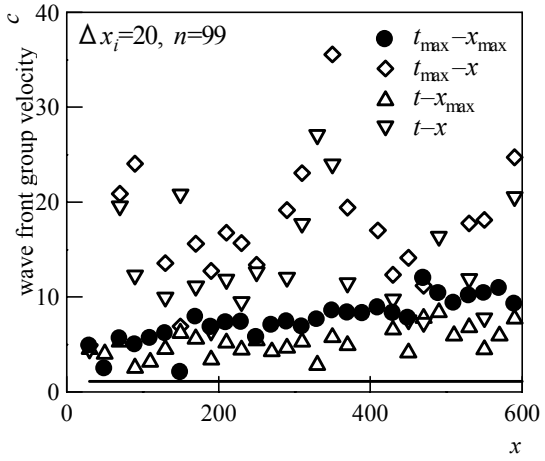

Fig. 13 Propagation velocity obtained from small amount of average vs. the wave motion coordinate x.

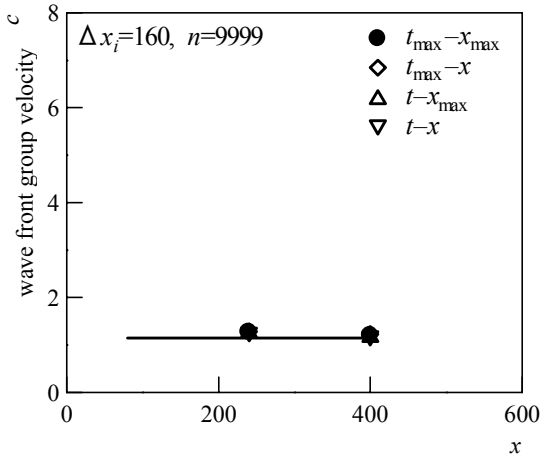

Fig. 14 Propagation velocity obtained from large amount of average relative to the wave motion coordinate x.

between the top and bottom figures of Fig. 4. We also investigated the disturbed density, pressure and total energy. The time developments of disturbed density and pressure are very similar to the one of the disturbed velocity but the total energy (Fig. 5) differs from them. However, a wave-like pattern can be found also in the total energy curve although it is not as clear as shown in the bottom two graphs of Fig. 4.

In order to know in which direction the wave propagates, we moved the rigid wall on the left hand side towards the upper right. As shown in Fig. 6, we can find no wave in the y direction but only small fluctuations. This result shows that the shear wave such as a distortional wave in solid [5] is not produced in a fluid even in the nano scale system. The wave propagates in the normal direction relative to the rigid wall surface.

Figures 7 and 8 show the second partial derivatives of the disturbed velocity with respect to time and space, respectively. They are also arranged from the top to bottom in the same manner as Figs. 4, 5 and 6. When the amount of average is small, fluctuations of the second partial derivatives are remarkable and the steep changes of the derivatives due to the arrival of the wave disappear in the fluctuations. On the other hand, if the large ensemble and long time averages are used, these steep changes come out clear as a maximum or a minimum value.

From Figs. 4, 7 and 8, we assembled the maximum values of the disturbed velocity and its second partial derivatives with respect to space and time, respectively, at the time close to arrival of the wave. They are shown in Fig. 9. They strongly depend on the amount of average when n is large. It can be supposed that the magnitude of the disturbance itself and its second partial derivatives with respect to space and time, respectively, will disappear when a huge amount of average is used.

We also investigated the disturbed density, pressure and total energy. They have very similar features to the disturbed velocity.

From these results, it can be concluded that if the amount of average is large, the peak values of physical quantities decrease and their temporal and spatial derivatives, respectively, also disappear. The degree of the decrease depends on the physical quantity and the amount of average.

The times of the maximum values in Figs. 7 and 8 correspond to the start of the abrupt increase of the disturbed velocity v_x as shown in Fig. 4. Therefore, we can find the wave front and the arrival time from Figs. 7 and 8. The times when $\partial^2 v_x/\partial t^2$ and $\partial^2 v_x/\partial x^2$ attain their maximums are not always identical. If the amount of average is large, this time difference will be very small as described later (Figs. 13 and 14).

3.2 Propagation velocities of the wave of dilatation and distortion

The propagation velocity of the wave can be experimentally obtained as a numerical value by measuring the arrival times of the wave front at each subregion. Figure 10 shows the relation between the positions of the center of subregion and the arrival times of the wave front there. In order to find the arrival time of the wave front, we used two ways, that is, $\partial^2 v_x/\partial t^2$ (Fig. 7) and $\partial^2 v_x/\partial x^2$ (Fig. 8) values. The marks ○ denoting $\partial^2 v_x/\partial x^2$ take positions along a slightly curved line. It can be supposed that they are located roughly on a straight line. Then, the wave front velocity c=1.138 is obtained. If the particles are argon atoms, the velocity is 873m/s and is close to a general sound velocity of 900~1500m/s for liquid. Therefore, it can be concluded that the value of 1.138 is the macroscopic propagation velocity. Let us call it a propagation velocity obtained from the wave front hereafter. On the other hand, the marks ● denoting $\partial^2 v_x/\partial t^2$ are scattered over a large value region. Therefore, the propagation velocity cannot be obtained from them. If a large amount of average is used, the marks ● are on a straight line as shown in Fig. 11. Then, we have wave group velocity c=1.049 and this value is very close to the previous one of 1.138. Because the velocities obtained from Figs. 10 and 11 are almost equal, it can be concluded that the propagation velocity obtained from the wave front is independent of the amount of average except for the very small amount of average.

The propagation velocity is also obtained from the mechanical property of the liquid, i.e. Eq. (2). Figure 12 shows the relation between density and pressure obtained for the case of Δx_i=160 and n=9999. Although, the relation is not exactly linear, it is approximated as a linear one shown by a straight line. Then we extrapolate c=1.009 from the estimation of p by the upper linear dependence. This value is also close to 1.138.

The macroscopic propagation velocity is also calculated in other way i.e. by the wave equation (1) in the continuum mechanics. We find first the times when $\partial^2 v_x/\partial t^2$ and $\partial^2 v_x/\partial x^2$ attain maximum or peak around the arrival time of the wave and then obtain the values of $\partial^2 v_x/\partial t^2$ and $\partial^2 v_x/\partial x^2$ at the times. This makes four values i.e.

$$(\partial^2 v_x/\partial t^2)_{\max} \quad : t = t_{(\partial^2 v_x/\partial t^2)_{\max}} \tag{12}$$

$$(\partial^2 v_x/\partial t^2) \quad : t = t_{(\partial^2 v_x/\partial x^2)_{\max}} \tag{13}$$

$$(\partial^2 v_x/\partial x^2)_{\max} \quad : t = t_{(\partial^2 v_x/\partial x^2)_{\max}} \tag{14}$$

$$(\partial^2{}_x v/\partial x^2) \quad : t = t_{(\partial^2 v_x/\partial t^2)_{\max}} \tag{15}$$

Combining four values, we have four kinds of propagation velocities i.e. {Eq. (12)÷Eq. (14)}$^{1/2}$, {Eq. (12)÷Eq. (15)}$^{1/2}$, {Eq. (13)÷Eq. (14)}$^{1/2}$ and {Eq. (13)÷Eq. (15)}$^{1/2}$ which are shown by marks ●, ◊, Δ and ∇, respectively, in Figs. 13 and 14. The horizontal lines in the figures show the values obtained previously from the wave front. For the case of small amount of average, the

values shown by marks ◊, Δ and ∇ are considerably scattered but ones shown by marks ● have almost the same value (Fig. 13). However, the points marked by ● are remarkably far from the straight line. The propagation velocity obtained by the small amount of average is very large. It can be concluded that ∂x and ∂t in the wave equation (1), which have been approximated by the finite difference elements with gradually decreasing size, are not respectively identical with an infinitesimally small length and time used in Taylor's series. Therefore, ∂x and ∂t are finite from the physical point of view.

As shown in Fig. 14, if a large amount of average is used, the difference among the values of marks ●, ◊, Δ and ∇ decreases and these marks approach to the straight line. It can thus be said that the disturbed velocity defined in the continuum mechanics is averaged with respect to particle in a region and time in the MD system.

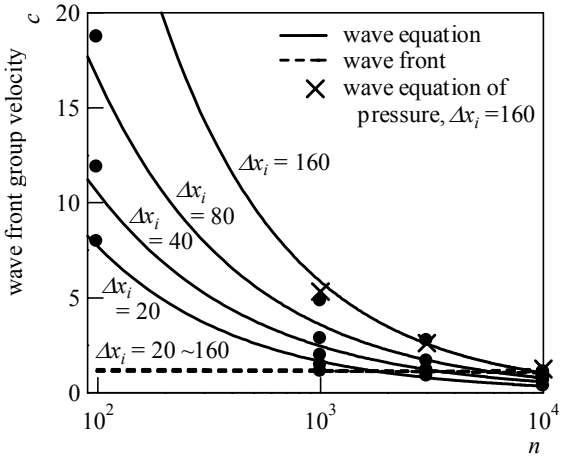

Fig. 15 Relation between propagation velocity of wave of disturbed velocity and space and time averages.

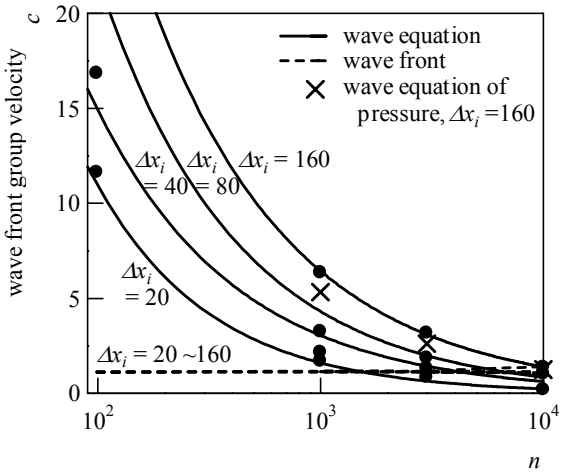

Fig. 16 Relation between propagation velocity of wave of disturbed density and space and time averages.

Figure 15 shows the effect of the amount of average on the propagation velocity obtained by the wave equation. The horizontal broken line indicates the propagation velocity obtained from the wave front. If a large subregion, that is, a large space average is applied together with the small time average, the propagation velocity obtained from the wave equation differs from that one of the wave front. In addition to this space average, if the time average increases, then the propagation velocity is close to one marked by the horizontal broken line. When a long time average over n=10000 is used, the propagation velocity deviates from the horizontal broken line again. The reason is not clear at the present time. In order to make a value close to the propagation velocity obtained from the wave front, it is necessary to select an appropriate time average for a certain space average.

Figure 16 shows the effect of the amount of average on the propagation velocity of the disturbed density obtained by the wave equation in the same manner as the disturbed velocity wave. We have the result that is similar to the disturbed velocity wave.

The marks × in Figs. 15 and 16 show the case of the disturbed pressure obtained from several numerical experiments when Δx_i=160. The results are also very similar to the cases of the disturbed velocity and the disturbed density.

Figure 17 shows the case of the total energy which can not be expressed by Eq. (1) along with the potential and kinetic energies obtained from several numerical experiments when Δx_i=160. Their results are also very similar to the cases of the disturbed velocity and the disturbed density.

Kotake concluded that the MD system can not explain non-equilibrium and/or unsteady state macroscopic phenomena if it has no local uniformities as described in the introductory section. It can be expected that if a large amount of average is used, the

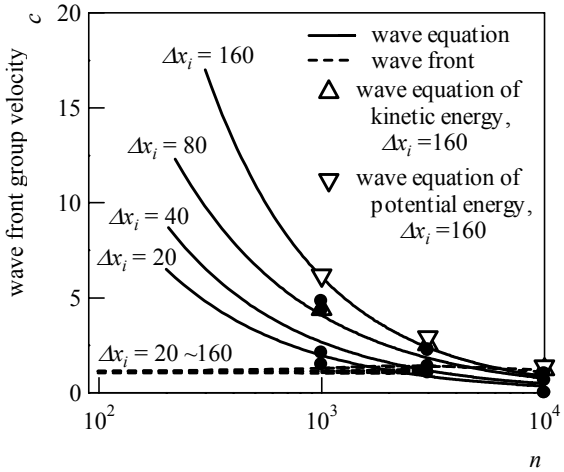

Fig. 17 Relation between propagation velocity of wave of disturbed energies and space and time averages.

physical quantities become locally equilibratory and locally uniform. However, Figs. 15, 16 and 17 show that the propagation velocity obtained from the wave equation does not approach to one obtained from the wave front motion only by increase in the amount of average. The propagation velocity obtained from the wave equation is identical with the one from the wave front when a long time average is used for a large ensemble and a short time average for a small ensemble. It is necessary to select an appropriate combination of time and space averages relative to a particle system being studied. This conclusion is the same as in the case of propagation of the disturbed displacement in an elastic solid continuum [5].

The present calculation of the wave front motion in liquid has been done for the case of two-dimensional (2D) sample. In order to validate our conclusions obtained in 2D reduction for the case of three-dimensional calculations, one has to take into account the force nature between particles and two-body approximation of LJ potential. Presence of neighbors in the third dimension will cause the interaction potential of each particle to be approximately 20 to 30% deeper compared with 2D one. The individual particle motions will also change velocity characteristics. However, change will be localized mostly in the vibrational motion of each particle and system averages used in this study will be applicable and valid for the 3D system. Wave front propagation in 3D particle medium as well as in 2D one is a one-dimensional simultaneous motion of perturbation of some values, spatially and temporally localized within several layers normal to the wave motion. With deeper potential and shorter bonds at the same values of temperature and pressure in the system as compared with the 2D case, the 3D calculation will show a higher rate of perturbation exchange in the unit of time between layers normal to direction of wave front motion. It will result in the increase in the amplitude of perturbation of around 10 to 15%, in our estimation. The group velocity of the wave as a collective process should be affected less by the depth of the particle bonds, the shift of the values in some 10% margins can be expected as we have seen in a pressure estimation compared for two-body and three-body potentials. Exact values can be obtained only by direct 3D calculations, though the dependencies obtained for the wave front motion should remain similar in the 2D and 3D evaluations.

4 Conclusion

In summary, the question whether and at what conditions the wave equation in the continuum liquid can be precisely described by particle motions in the MD system has been answered positively and conditions have been clarified. For a given system of particles of defined size and population of species, if an appropriate spatial and temporal average value of particle motion can be defined, the averaged characteristics of motion under condition of wave propagation correspond to the wave equation of the continuum mechanics. Relating to the size of the MD model, the spatial region average as it was shown should be directly proportional to the average size of time interval. Such wave behavior was confirmed for the propagation of the velocity, density, and pressure disturbance wave, as well as for the energy disturbance wave. Then, the wave propagation velocity can be extracted from the continuous wave equation. For two-dimensional Ar model, obtained values of c in interval from 1.138 to 1.009 are close to general sound velocities in liquid.

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