Why does not expansion shock wave exist in nature?

Nobuyoshi Komatsu and Takashi Abe

JAXA/The Institute of Space and Astronautical Science, Yoshinodai 3-1-1, Sagamihara, Kanagawa, Japan

Abstract. Why does not expansion shock wave exist in nature? The reason for this is widely believed to be the irreversibility in nature while the clear confirmation for this belief is not yet accomplished. In order to resolve the question from a microscopic viewpoint, an implosion process dual to an explosion process was investigated by means of the molecular dynamics method. To this aim, we employed a 'bit-reversible algorithm (Bit MD)' which is completely time-reversible in a microscopic viewpoint and is free from any round-off error. Here we show that, through a dual implosion simulation (i.e., a time-reversible simulation of the explosion), the expansion shock wave is successfully formed in the Bit MD simulation. Furthermore, we show that when the controlled noise is intentionally added to the Bit MD, the expansion shock wave disappears dramatically and turns into an isentropic expansion wave, even if the noise is extremely small. Since the controlled noise gives rise to the irreversibility in the Bit MD simulation, it can be concluded that the irreversibility in the system prohibits the expansion shock wave from appearing in the system.

Keywords: Irreversibility, Expansion shock
PACS: 47.40.-x, 52.35.Tc, 52.57.Fg

INTRODUCTION

Shock waves are a phenomenon of frequent occurrence in a variety of fields, from a supersonic aircraft to a supernova explosion. Such a shock wave is a so-called '*compression* shock wave' which compresses a propagation medium after the shock wave passage. On the contrary, it seems that a so-called '*expansion* shock wave', through which a propagation medium expands and becomes less dense while keeping its discontinuity like an ordinary compression shock wave, does not exist in nature especially for a 'gaseous' medium. (Although, as predicted by Zeldovich [1], an expansion shock wave can be generated in the vicinity of the 'liquid-vapor' critical point [2, 3, 4], it does not exist in a 'gaseous' medium.)

In fact, it is widely believed that, because of the second law of thermodynamics (i.e., the law of entropy increase) or the irreversibility in nature, we cannot observe the expansion shock wave in nature for a 'gaseous' medium. However, to our knowledge, there is no clear evidence for that at least from a microscopic viewpoint.

The expansion shock wave can be possible at least in a 'thought experiment', if we assume that the gas dynamic behavior can be composed of motion of molecules in the gas and the molecular motions are 'time-reversible'. It seems that this assumption is generally accepted [5, 6, 7]. To illustrate the possibility of the expansion shock wave, we will focus on the duality of explosion and implosion processes. That is, we consider an implosion process which can be generated by the time-reversal operation applied, at a certain time, to the ordinary explosion process. In this sense, this imploding process is dual to the explosion process. In the time-reversal operation, velocities of all particles in the gas are reversed instantaneously. In the explosion process, we will see a shock wave propagating outwards. On the other hand, we will see, in the dual implosion process, the shock wave propagating reversely (i.e., inwards in spatial direction), if all the molecules behave in a completely time-reversible manner. In such a shock wave, the propagation medium must expand after the shock passage. Therefore such a shock wave must be the expansion shock wave. Then, a question arises: 'Does a law of nature permit such a process?' or, 'If not, how such a process can be avoided in nature?' In the present paper, we will answer the question investigating this problem from a microscopic point of view.

In order to answer the question and to study the expansion shock wave from a microscopic viewpoint, a molecular dynamics method (MD) is quite suitable. Nevertheless, the expansion shock wave so far has not been investigated by means of the MD methods, although the compression shock wave has been extensively studied [8, 9, 10]. We can guess that the reason for this is the irreversibility unavoidable in the standard MD methods, since our previous study based on the 'bit-reversible algorithm' for the MD method and a 'controlled noise' with it[11, 12], revealed that the standard MD methods can not avoid a numerical 'irreversibility' which is root-caused by the round-off error in the numerical operation for the floating-point real number. Because of this numerical irreversibility, the standard MD methods are not suitable for the investigation of the expansion shock wave from a microscopic view point. On the other hand, the bit-reversible algorithm (Bit MD), which was developed by Levesque and Verlet, is known to be free from any round-off error and is completely time-reversible [13] and enables us to introduce the effect of the irreversibility in a controlled fashion[11, 12]. Therefore, instead of the standard MD, we will employ the Bit MD for the present investigation. This technique will enable us to get some insight how the expansion shock wave is formed in the present implosion process and to clarify the effect of the irreversibility on it.

The present paper is organized as follows. In Sec. II, we give a brief review of the MD techniques including the bit-reversible algorithm, in order to simulate an implosion process dual to an explosion process. In Sec. III, we investigate how the expansion shock wave is formed in the implosion process and discuss the effect of the irreversibility on it. Finally, the conclusion is given.

MD TECHNIQUES

To make the present paper self-consistent, we will first give a brief review on Bit MD [13, 11, 12]. Now, we will consider a system of N particles of mass m enclosed in a cubical box of size L which is discretized into small cubical sub-cells. It is assumed that particle locations are discretized in that any particle resides on the vertexes of the cubical sub-cells. The minimum lattice distance ΔL $(= L/M)$ or the size of the cubical sub-cell, by which the coordinate space is discretized, is defined as the side length of the cubical box L divided by some integer value M. Although we can choose any integer value M, the maximum value is 2^n if n-bit integers are employed for the computation. Because of this discretization, the position of a particle in the discrete coordinate system is represented by integers. In this context, the equation of motion for the particles in the discrete coordinate system can be written as

$$\begin{aligned} \frac{\partial^2 X_i}{\partial t^2}(\Delta t)^2 &= X_i(t+\Delta t) - 2X_i(t) + X_i(t-\Delta t) \\ &= \sum_j \left[\left(\frac{f_{ij}(t)}{m} \right) \frac{(\Delta t)^2}{\Delta L} \right]_{\text{Integer}} \end{aligned} \tag{1}$$

where $f_{ij}(t)$ is a partial force exerted by the *j-th* particle on the *i-th* particle locating at position X_i at a time t. The term in the summation on the right hand side of Eq. (1) is calculated based on the particle locations, and the value in the bracket $[\ ]_{\text{Integer}}$ is converted to an integer since, in general, the value calculated in this way is not in integer but in real number. Because of both the space discretization and this conversion process to integer, Bit MD keeps the time-reversibility and is free from any round-off error [13].

In the present study, we assume for simplicity the 2 dimensional system and integrate a set of classical equations of motion for the particles interacting through the Lennard-Jones potential $\phi(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ with a cut off radius r_c of $2^{1/6}\sigma$, in order to mimic particles in gas (i.e., we employ the 'repulsive' L-J potential.). Here, the constants, σ, ε, m, ε/κ_B, $\sigma(m/\varepsilon)^{1/2}$ are chosen, respectively, as units of length, energy, mass, temperature and time, where κ_B is Boltzmann's constant.

For simulating an explosion process by means of the MD method, an initial 'hot droplet' and 'background gas' around it are prepared. In the present study, they can be prepared by cutting out a droplet from a thermally equilibrated periodic system as follows [14, 15, 16]. In a square cell, N_{eq} particles are equilibrated under periodic boundary conditions at a target temperature and number density by using the temperature control technique. From the inner region of this equilibrated system, the initial hot droplets are generated by cutting out N_d particles included in a circular region of a radius r_d. The low density background gas with the target temperature and number density is similarly produced, except that the particles inside a circular region of a radius r_d are removed from the center of the square cell. Finally, the particles prepared for the hot droplet are immersed in the hole of the background gas in the square cell. The background gas together with the hot droplet immersed in the hole forms the initial setup for the simulation. The number density ρ, temperature T and number of particles in the hot droplet are set to be 0.80, 3.0, 3600, respectively. As for the background gas, they are set to be 0.08, ~ 0.0, 7891, respectively. Accordingly, the total number of particles N becomes 11491.

To simulate the explosion process under a restriction of 'constant energy', the set of equations of motion is integrated by using Bit MD with Δt =0.005 as the time increment for the integration. The total number of time-steps is set to be 4000; i.e., the terminating time for the simulation of the explosion process is set to be $t_{\text{Ex}} = 20$. Even though the periodic boundary conditions are imposed at the boundaries of the square cell and may affect adversely the simulation result, we try to avoid the adverse effect by using a sufficiently large square cell. To this aim, the cell length L is set to be 320σ. For this size of the cell and the present simulation time period of $t_{\mathrm{Ex}} = 20$, the boundary effect does not propagate to the explosion area of our interest and, therefore, the explosion process is not affected by the boundary conditions. Note that the adverse effect caused by the discretization of the coordinate for the particles is small enough to be neglected from a physical point of view [11, 12, 13]. In the present study, the minimum lattice distance ΔL for the 30bit-integers for the present Bit MD simulation is $3 \times 10^{-7}\sigma(= L/M = 320/2^{30})$, and is extremely small even compared with the particle diameter, 1σ.

RESULTS

When the explosion simulation starts, the initial hot droplet rapidly expands compressing the background gas as shown in Fig. 1. This compression generates the shock wave propagating outward in the background gas as shown in Fig. 2. We have confirmed that the explosion simulation generates a discontinuous surface corresponding to the so-called compression shock wave, as reported in the past works [8, 9, 10, 17, 18, 19].

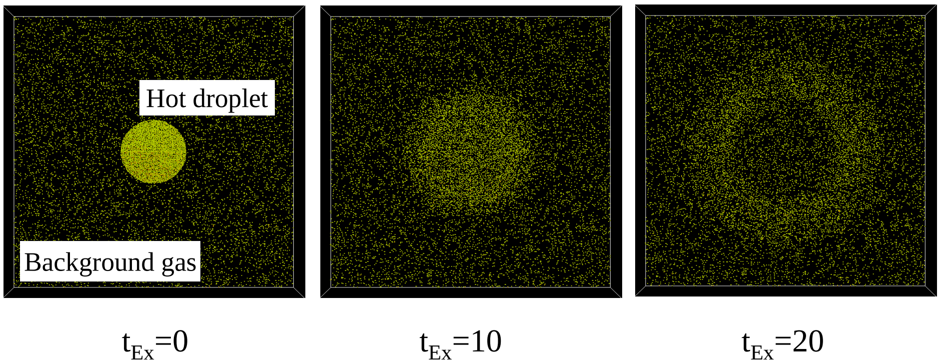

FIGURE 1. Snap shots of the explosion simulation by the molecular dynamics method. The locations of the particles are depicted by dots. As soon as the simulation starts, the initial hot droplet starts to expand and the high density region corresponding to a compression shock wave propagates outwards.

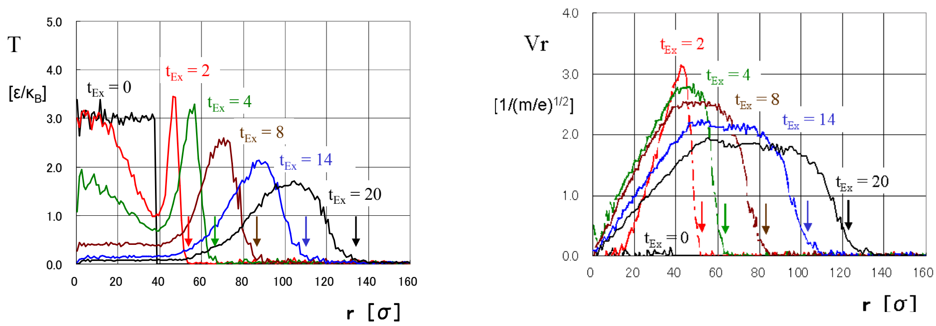

FIGURE 2. Temporal variation of the radial profiles for temperature and radial velocity. The shock location is indicated by an arrow in each profile.

In order to simulate the implosion process in the Bit MD method, we make use of the explosion simulation result at the final time (i.e., $t_{\mathrm{Ex}} = 20$) and apply a time-reversal operation on it. For the time-reversal operation, the initial positions and velocities of the particles are set to be the ones at $t_{\mathrm{Ex}} = 20$ in the explosion simulation except that all the particles reverse their velocities. Taking this setup as a initial condition, the implosion simulation starts. Then, it is expected that the shock wave turns into the expansion shock wave in this simulation, since the Bit MD simulation is completely time-reversible and, therefore, we can expect that all the profiles vary reversely except V_r changing its sign from positive to negative.

The radial profiles of the temperature and radial velocity in the implosion simulation are shown in Fig. 3. In these figures, the profiles of the temperature and radial velocity at t_{Im}=6, 12, 16, 18 and 20 correspond to the ones at t_{Ex} =

$14,8,4,2$ and 0 in the explosion simulation, respectively. Note that $t_{\rm Ex}$ is an elapsed time from the initial state for the explosion and, on the other hand, $t_{\rm Im}$ is an elapsed time from the initial state for the explosion, in other words, the state at $t_{\rm Ex}$=20 for the explosion with the time reversal operation. The horizontal axis represents the radial distance from the center of the hot droplet at the initial state of the explosion simulation. In those figures, the profiles in sold line are the result by the time-reversible Bit MD simulation. As we expect, each profile is exactly equal to the corresponding profile of the explosion process since every particles move back exactly. Only exception is that the velocity reverses its direction. That is, since the process is an implosion, the medium implodes inwards. The shock wave observed in the explosion process propagates, instead, inwards keeping its characteristics of discontinuity. Therefore, this wave is a kind of shock wave. After passage of the discontinuous wave, the propagation medium is suddenly decelerated to zero velocity and the temperature suddenly decreases. In other words, this shock wave is an expansion wave. Since the propagation medium expands after the passage of the shock wave, we can conclude that the expansion shock wave is formed in the implosion simulation by Bit MD.

In our earlier papers[11, 12], we have demonstrated that the controlled noise can give rise to an irreversible nature in the Bit MD simulation and have examined in detail the effect of the controlled noise on the irreversibility. In fact, we found that even a negligibly small controlled noise can give rise to the irreversibility. Roughly, the more intense the controlled noise is, the more effectively the irreversibility appears. On the other hand, the effectiveness of the irreversibility is saturated with increasing the intensity of the controlled noise. Therefore, by adding some controlled noise in the present simulation, we can examine an effect of the irreversibility on the expansion shock wave quantitatively. The present controlled noise is a deliberate displacement of the particles; that is, the particles suffer displacement of their position suddenly by a certain amount, in a random direction. Here, the 'quantity' of the noise is controlled by the following three ways [11, 12]:

1. The magnitude of the displacement, $dX_{\rm cn}$.
2. The frequency of its addition, $F_{\rm cn}$.
3. The number of particles added with the displacement, $N_{\rm cn}$.

To parametrically control the intensity of the noise, we vary the number of particles affected by the noise; i.e., $N_{\rm cn}/N$ is set to be 0%, 1%, 10% or 100%, where N represents the total number of particles. On the other hand, $dX_{\rm cn}$ and $F_{\rm cn}$ are fixed; i.e., the magnitude of the displacement $dX_{\rm cn}$ is set to be $1[\Delta L]$, and the frequency of its addition $F_{\rm cn}$ is for every time step. Note that the magnitude of this displacement is the minimum among the possible ones and is extremely small ($3\times10^{-7}\sigma$) compared with even the particle diameter, 1σ.

The effects of the controlled noise are also depicted in Fig. 3. As shown in these figures, the discontinuous surface or the expansion shock wave dramatically disappears due to the controlled noise, even in the case of $N_{\rm cn}/N$=1%; i.e., in the case of the minimum noise intensity. In fact, as seen at $t_{\rm Im}=12\sim18$ in Fig. 3a, the temperature and velocity profiles associated with the shock wave turn into other profiles dramatically. Even though the more intensive controlled noise is added to the implosion process, the behavior of the process is not influenced so much, as seen from the fact that the profiles for the case of $N_{\rm cn}/N$=1%, 10% and 100% are overlapping. That is, the behavior of the implosion process converges into a single one regardless of the 'quantity' of the noise. In other words, the behavior of the present implosion process is dramatically dominated by the fact that the controlled noise exits or not.

This dramatic modification of the flow in the case of the dual implosion process shows a sharp contrast to that in the case of the explosion process. That is, in the case of the explosion process, no such modification is induced by the controlled noise, which is consistent with the fact widely accepted.

Let us examine the behavior of the implosion process modified by the irreversibility from a macroscopic viewpoint. The region of expansion in the flow can be clearly identified as a region in the velocity distribution where the velocity recovers to zero from a negative peak value. In the behavior of the implosion process simulated by Bit MD *with* the controlled noise, the region of expansion becomes more diffusive compared to the one simulated by Bit MD *without* the controlled noise. Furthermore, the diffusive expansion region in the former becomes more diffusive as time goes on (until $t_{\rm Im}=16$), while the one in the latter keeps its form and remains to be discontinuous since it is the expansion shock wave. Therefore, we can interpret the diffusive expansion region as a so-called isentropic expansion wave. This behavior of the implosion process is natural from a viewpoint of macroscopic fluid dynamics.

The results presented so far are based on the assumption that the molecular motion is governed by the classical equation of motion influenced by some numerical noise. First of all, we must recall that this assumption may have an essential difficulty because, in general, microscopic laws are based on quantum mechanics in which an observable in the Schrödinger equation is time-reversible and, therefore, it seems that the difficulty to explain the macroscopic irreversibility based on the reversible microscopic equation, still exists. However, according to Nelson [20], the basic equation for the quantum mechanics can be formulated by a new stochastic differential equation; i.e, Nelson's equation, which combines the classical Newton's law with the quantum random force. That is, his approach to the quantum mechanics suggests that there is a possibility for the classical dynamics to be applicable not only to the macroscopic system but also to the microscopic system when an appropriate quantum noise is assumed. According to his theory, the uncertainty of the particle trajectory can be estimated as,

$$\delta x \sim \sqrt{\frac{\hbar}{2m}\delta t} \tag{2}$$

where δt is a time increment for Nelson's equation and δx is a quantum noise corresponding to δt. As a matter of fact, Eq. (2) gives 4.1×10^{-12}m when we assume Argon and $\delta t = \Delta t$, while the magnitude of the present numerical noise, ΔL, is as small as 2.5×10^{-17}m for Argon. That is, the present numerical noise is sufficiently smaller even as compared to the quantum noise. Therefore the irreversibility in the present study is not caused by unphysically large numerical noise and, in this sense, the present assumption may be reasonable.

CONCLUSION

In order to study the characteristics of the expansion shock wave from a microscopic viewpoint, an implosion process dual to an explosion process was investigated by means of the Bit MD method. It was demonstrated that the expansion shock wave formed in the time-reversible simulation was quite sensitive to the noise added to the simulation. Since the noise added to the Bit MD simulation causes the irreversibility in the simulation, we can conclude that the irreversibility causes the disappearance of the expansion shock wave. Furthermore, the macroscopic flow behavior caused by the noise was independent of the 'quantity' of the noise. In other words, the behavior of the macroscopic implosion process is dramatically dominated by the fact that the controlled noise exits or not or, i.e., the irreversibility. This may correspond to the fact that the expansion shock wave does not exist in nature, and may verify a widely-believed fact that, because of the second law of thermodynamics, we cannot observe the expansion shock wave in nature.

REFERENCES

1. J. Zeldovich, Zh. Eksp. Teor. Fiz., **16**, 363(1946).
2. A.A. Borisov, Al.A. Borisov, S.S. Kutateladze and V.E. Nakoryakov, J. Fluid Mech. **126**, 59(1983).
3. N.M. Bulgakova, Phys. Rev. E **60**, R3498(1999).
4. N.M. Bulgakova, I.M. Bourakov and N.A. Bulgakova, Phys. Rev. E, **63**, 046311(2001).
5. J.L. Lebowitz, Physics Today, **46(9)**, 32(1993).
6. W.G. Hoover, *Time reversibility, Computer simulation, and Chaos*, World Scientific, Singapore, 1999.
7. J.E. Broadwell, J. Stat. Phys. **103**, 1125(2001).
8. W.G. Hoover, Phys. Rev. Lett. **42**, 1531(1979).
9. B.L. Holian, W.G. Hoover, B. Moran and G.K. Straub, Phys. Rev. A **22**, 2798(1980).
10. E. Salomons and M. Mareschal, Phys. Rev. Lett. **69**, 269(1992).
11. N. Komatsu and T. Abe, Physica D **195**, 391(2004),
12. N. Komatsu and T. Abe, Comput. Phys. Comm. **171**, 187(2005).
13. D. Levesque and L. Verlet, J. Stat. Phys. **72**, 519(1993).
14. N. Komatsu and T. Abe, Phys. Rev. E **72**, 021601(2005).
15. A. Vicentini, G. Jacucci and V.R. Pandharipande, Phys. Rev. C **31**, 1783(1985).
16. A. Strachan and C.O. Dorso, Phys. Rev. C **55**, 775(1997).
17. T.E. Itina, J. Hermann, P. Delaporte and M. Sentis, Phys. Rev. E **66**, 066406(2002).
18. F. Garrelie, J. Aubreton and A. Catherinot, J. Appl. Phys. **83**, 5075(1998).
19. P. Gaspard and J. Lutsko, Phys. Rev. E **70**, 026306(2004).
20. E. Nelson, Phys. Rev., 150(1966)1079.

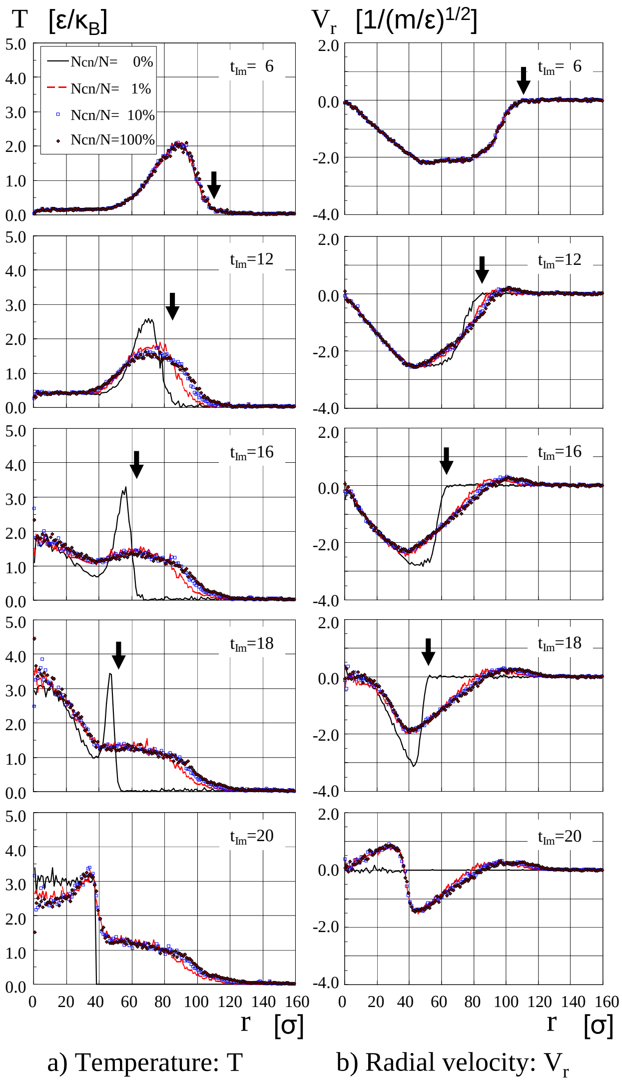

FIGURE 3. Radial distributions of the temperature and radial velocity in the implosion process. The left and right figures represent a) temperature and b) radial velocity, respectively. N_{cn}/N represents a quantity of the controlled noise added to the simulation. Here, N_{cn}/N=0% (i.e., *without* noise) is the time-reversible Bit MD simulation result. The arrow in each figure represents a shock front of an expansion shock wave in the case of N_{cn}/N=0%. As time goes on (i.e., from top figures to bottom figures), the medium propagates inwards. In the case of N_{cn}/N=0%, a discontinuous surface corresponding to a expansion shock wave is formed. However, the expansion shock wave suddenly disappears due to the controlled noise, even in the case of N_{cn}/N=1%. Note: The temperature and radial velocity at the radial position r are the ones averaged over circumferentially. All the results are averaged over 10 simulations with the identically-prepared initial setup.