Shock-like and Detonation-like Waves in One-dimensional Lattice Chains

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1 Introduction

Beginning with Schrödinger's study in 1914, there has been interest in understanding the dynamics and structure of shock waves in one-dimensional lattices or chains.[1] While a chain interacting with a linear force potential (harmonic oscillator) does not exhibit shock-like waves (i.e., wave speed is independent of wave amplitude), nonlinear lattices do exhibit a spectrum of interesting dynamics dominated by the dispersive nature of the lattice (e.g., solitons). Piston-driven shock-like waves were studied extensively from the mid-1960's to the early 1980's in the pioneering years of computational molecular dynamics simulations [2-4] as reviewed in [5]. The dynamics of shock waves in nonlinear chains was found to be in close, but not exact, agreement with the traditional Rankine-Hugoniot relations.[4] Detonation-like waves (i.e., shock-like waves with the potential to release energy stored in the lattice) have received relatively little attention beyond the study of [6]. As a first step, it is of interest to explore systems that can be shown to revert to classical shock and detonation phenomena, in other words, systems that exhibit shock and detonation waves that agree with the classical Hugoniot and Chapman-Jouguet relations.

While one-dimensional systems offer a tremendous advantage in terms of simplicity of modeling and analysis, a one-dimensional gas comprised of "beads on a wire" results in trivial behavior in which each particle in collision with its neighbor simply transfers its velocity to the neighbor and there is no thermalization toward a Maxwellian distribution of particle velocities. A piston moving at speed v into a gas of initially quiescent elastic spheres, for example, will result in a front moving at speed $2v$, leaving particles alternating between velocity $2v$ and 0 in its wake. This lack of thermalization prevents a temperature from being defined and, in turn, the system cannot be shown to be equivalent to the continuum-based conservation laws. Such a "pathological" one-dimensional system is geometrically constrained such that particle motion cannot be randomized into the most probable configuration (as is the case in two- and three-dimensional gases).

Recently, however, it has been found that one-dimensional chains with two different masses do undergo a thermalization process, albeit at a slower rate than in a two- or three-dimensional gas.[7] The different masses of the particles permit sufficient randomization of the dynamics to result in a relaxation to a Maxwellian distribution of particle velocities, albeit the relaxation can be quite slow in comparison to more familiar two- and three-dimensional gases. The present study uses this system (namely, a one-dimensional chain of alternating masses) to show the equivalence between a molecular-

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dynamics based approach and the more traditional continuum models. This is done for both inert problems (shock waves) and with energy release (detonation waves). Sirmas and Radulescu recently demonstrated detonation-like waves in a two-dimensional hard-disk gas with energy release upon sufficiently energetic collisions.[8] This study attempts to reproduce similar phenomena in an even simpler system (one-dimensional gas).

2 One-Dimensional System

The system considered here is a chain of point-like masses sliding along a frictionless wire that only interact via perfectly elastic, instantaneous collisions (i.e., hard-core potential). The masses have an average mass of unity, however, to prevent the trivial behavior of one-dimensional systems, the masses alternate between values equally off-set from unity (e.g., 0.5, 1.5, 0.5, 1.5, etc.). The masses are initially located one unit apart and initialized with unity velocity (one unit space per unit time) in either the positive or negative direction with equal probability, as assigned by a random number generator. Thus, the initial velocity distribution function consists of two δ-functions located at $v = -1$ and 1.

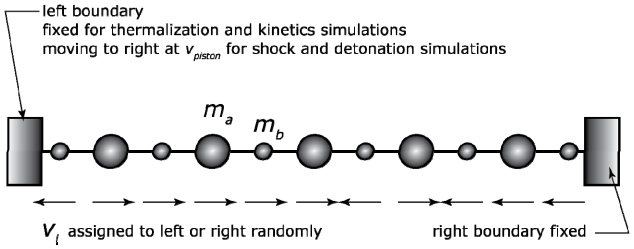


Figure 1. A system of elastic particles, alternating in mass m_a and m_b, on a frictionless wire, initialized with velocity v_i to left or right.

If a system is initialized in this way (with elastic "bumpers" confining the particles at each end of the domain), the dynamics can be solved for by an event-driven molecular dynamics simulation, and the statistics on the distribution of particle velocities can be collected. The result of such a simulation with 100,000 particles with alternating masses (1.5, 0.5) is shown in Fig. 2(a), and compared to the expected Maxwell-Boltzmann (M-B) distribution of a one-dimensional system

$$f(v) = \sqrt{\frac{m}{2\pi kT}} \exp\left[-\frac{mv}{2kT}\right] \tag{1.1}$$

where the temperature of the system is calculated by using the initial total kinetic energy of the system which is assumed to be shared by each particle upon reaching equilibrium according to

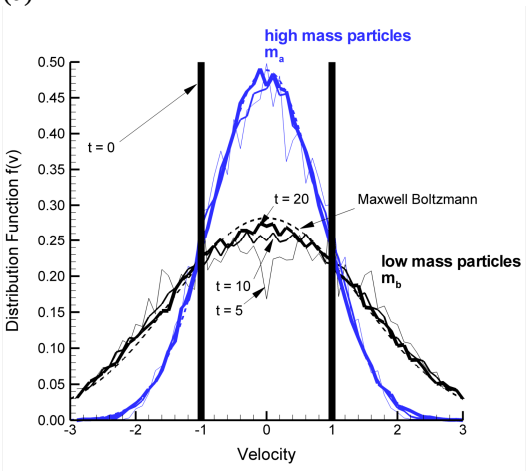
$$E_{tot} = \frac{1}{2} n_{particles} kT = \sum_{i=1}^{n_{particles}} \frac{1}{2} m_i v_i^2 \tag{1.2}$$

where the Boltzmann constant has been set to unity (note that there is only one degree of freedom in a one-dimensional system). The simulation appears to relax to the M-B distribution on a timescale of approximately 10 time units (corresponding to approximately 5 collisions on average per particle). The value of the probability function measured at the most probably velocity ($v = 0$) as a function of simulation time is shown in Fig. 2(b). In order to quantify the relaxation to M-B statistics, a relaxation time τ_r is defined as being when the value of the distribution function for the most probable velocity is within $\frac{1}{e}$ of the M-B value.

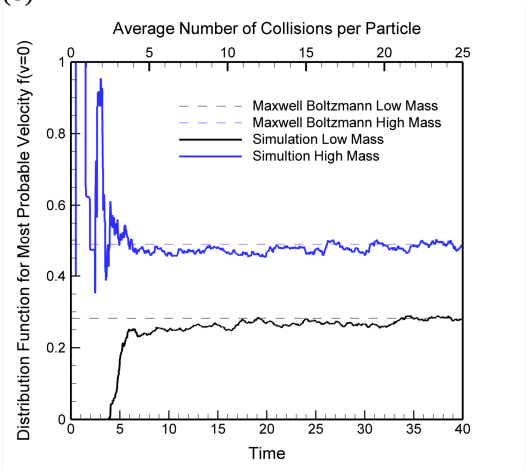
Following Hurtado [7], the relaxation time τ_r for systems with varying mass ratio $\beta = \frac{m_a}{m_b}$, constraining the average mass to always be unity, was studied systematically. Systems with particle masses from

(1.92, 0.08) to (1.1, 0.9) were studied, and the relaxation time measured, as shown in Fig. 2(c) for both the heavy mass (large symbol) and lighter mass (mass symbol). It is seen that systems with very similar masses (e.g., m_a, m_b = 1.1, 0.9, giving $\beta = 1.222$) are slow to thermalize, as well as the greater mass particles in systems with very dissimilar masses (e.g., m_a, m_b = 1.92, 0.08, $\beta = 24$). The small mass ratio systems are apparently not sufficiently randomized by the collisions to quickly thermalize, while the larger masses are slow to respond to collisions from their small mass neighbors. For the remainder of this study, we will use a system of $\beta = 3$ (m_a, m_b = 1.5, 0.5), since both particles thermalize at approximately the same timescale.

(a)



(b)



(c)

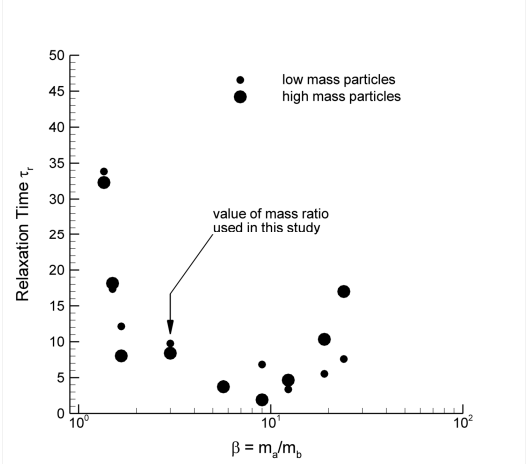


Figure 2. (a) Velocity distribution function for a system of 100,000 masses (alternating mass 1.5, 0.5) at different times, showing relaxation to M-B statistics. (b) Value of distribution function for most probably velocity Rate of reaction in a one-dimensional chain of elastic particles with a critical collision energy required for reaction to occur. Symbols are simulation results and lines are from the Arrhenius expression (1.5). (c) Relaxation time for the low mass (small symbols) and high mass (large symbols) particles as a function of the particle mass ratio $\beta = m_a/m_b$.

This study also considered multiple mass systems (with up to 10 different masses) and different methods of initialization (randomly sequenced masses, rather than alternating), however, the dynamics did not significantly change and no particular system was found to thermalize significantly faster than those in Fig. 2 (i.e., all systems required on the order of 5 to 10 collisions per particle to thermalize).

3 System with Energy Release

Energy release can be introduced into the collisions of a hard-sphere potential gas to simulate the effect of an energetic chemical reaction. A threshold collision energy that is required to initiate reaction can be defined using the reduced mass and the relative velocity:

$$E_{col} = \frac{1}{2}\mu\left(v_a - v_b\right)^2 \tag{1.3}$$

where μ is the reduced mass $\mu = \frac{m_a m_b}{m_a + m_b}$. For collisions that exceed this energy, kinetic energy is added to the particles while total momentum remains constant as follows:

$$v_a' = \frac{m_a^2 v_a \pm \sqrt{m_a m_b\left(2E_{in}(m_a + m_b) + m_a m_b (v_a - v_b)^2\right)} + m_a m_b v_b}{m_a(m_a + m_b)} \tag{1.4}$$

where "+" is used for $v_a < v_b$ and "–" for $v_a > v_b$. For collisions of lesser energy, the collisions are the traditional elastic collision (i.e., velocity of approach equals velocity of departure). This collision energy threshold is the molecular origin of the activation energy concept invoked in Arrhenius kinetics models.

From collision theory of reactive hard-sphere molecules [9], the rate of reactions between *A* and *B* is given by an Arrhenius-type expression

$$Z_{AB} = \overline{|v|}\frac{n_a}{l_x}\frac{n_b}{l_x} p \exp\left[-\frac{E_a}{RT}\right] \tag{1.5}$$

where the average particle speed is given by $\overline{|v|} = \sqrt{\frac{2kT}{\pi\mu}}$. The particle density terms $\frac{n_a}{l_x}, \frac{n_b}{l_x}$ are unity, since the particles initially have unity spacing. The E_a term is the activation energy, which is set equal to the critical energy to initiate reaction, and the *p* term is a steric coefficient that represents the probability that a given collision with sufficient energy will actually result in a reaction.

In order to compare the predicted reaction rate of (1.5) to the actual rate of reactions, simulations were performed at different initial temperatures (by varying the initial value of particle velocity) and statistics on the number of collisions were collected (the energy release was set to an arbitrarily low value, so that the energy release would not affect the temperature). The steric coefficient was set to unity for these simulations with 10,000 particles. The results are compared to the predictions of (1.5) in Fig. 3, and the agreement is seen to be nearly exact. This correspondence verifies that the critical collision energy is the activation energy of the reaction as used in the Arrhenius expression.

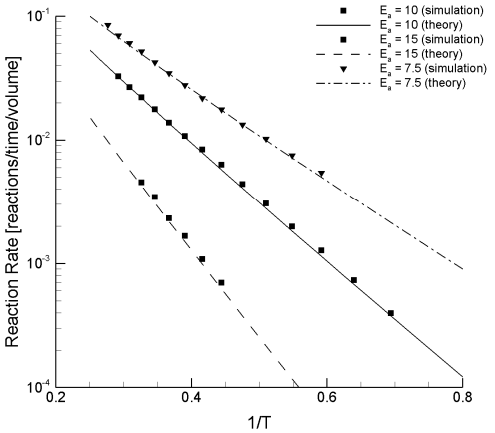


Figure 3. Rate of reaction in a one-dimensional chain of elastic particles with a critical collision energy required for reaction to occur. Symbols are simulation results and lines are from the Arrhenius expression (1.5).

4 Shock Waves

Shock waves were driven into the one-dimensional chain by imposing a constant velocity on the left-most particle. The shock velocity was measured in a chain of 1,000 particles that had previously been initialized by randomly assigned unity velocity (–1,1) and allowed to thermalize before the piston motion was started. Reaction was turned off for these simulations. The shock velocity was measured by recording its arrival time through the chain. For piston velocities greater than the initialization velocity of the chain, the shock was easily identified, as seen in Fig. 4. As the piston motion became on the order of the thermal motion of the particles, the shock could no longer be identified "by eye" and it was necessary to record the motion of particles in simulations without the piston and subtract off their motion for simulations with the piston in order to identify the shock front location.

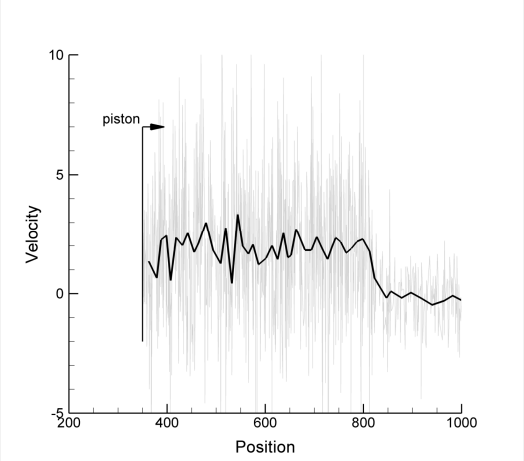


Figure 4. Snapshot of a simulation with a piston of velocity V_{piston} = 2 being driven into a chain of elastic particles previously allowed to come into equilibrium (grey: particle velocities; solid: velocity averaged over 20 particles).

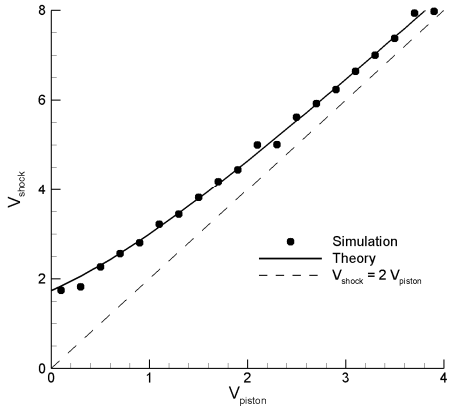


Figure 5. Velocity of shock measured with a piston of velocity V_{piston}. Solid curve is normal shock relations with γ = 3; dashed curve is wave velocity in uniform mass system (V_{shock} = 2 V_{piston}).

The measured shock velocities are shown in Fig. 5 and compared to the predictions of the normal shock relations of a perfect gas (i.e., Rankine-Hugoniot relations)

$$M_{shock} = \frac{V_{shock}}{c_o} = \frac{\frac{\gamma+1}{2}\frac{V_{shock}}{c_o} + \sqrt{\left(\frac{\gamma+1}{2}\frac{V_{shock}}{c_o}\right)^2 + 4}}{2} \tag{1.6}$$

Where the initial sound speed is given by $c_o = \sqrt{\gamma \frac{k}{m} T}$. The ratio of specific heats is given by $\gamma = \frac{\xi+2}{\xi}$ where ξ is the molecular degrees of freedom (ξ = 1 for one-dimensional gas). Also shown in Fig. 5 is the wave velocity that occurs in a uniform mass system, wherein each particle simply exchanges velocity upon collision. The simulations reproduced the shock relations, including recovering the predicted acoustic velocity ($c_o = \sqrt{3} \approx 1.732$) in the limit of zero piston velocity.

5 Detonation

Simulations were also performed with a piston (v_{piston} = 2.0) driving a shock into a system of 10,000 particles with reactive collisions (as in Section 3). For these simulations, E_{in} = 10 and the critical value of collision energy $E_{col} = E_a$ = 20. The steric factor p was given values between 0.05 and 1 for these simulations. For a value of p = 0.05 (i.e., only 5% of collisions with sufficient energy actually

result in a reaction), a wave propagating a quasi-steady velocity was observed (Fig. 6) with an average velocity within 2% of the detonation velocity predicted by the Chapman Jouguet relation

$$M_{CJ} = \frac{V_{CJ}}{c_o} = \sqrt{(\gamma+1)Q + \sqrt{((\gamma+1)Q+1)^2 - 1} + 1}\,; \quad Q = \frac{\Delta q}{c_p T_o} \tag{1.7}$$

The velocities of the individual particles are shown as grey in Fig. 6, for which identification of the wave structure is difficult due to large distribution of particle velocities. If the velocities of the particles are binned (with 100 particles per bin) and averaged, plotting the average velocity (heavy black line) shows a von-Neumann-like spike. The average number of reacted particle per bin is shown in red, and exhibits a ZND-like reaction zone structure. As the value of energy input increases, the measured detonation velocity increases as well, as shown if Fig. 7, in good agreement with the predictions of (1.7). For large values of E_{in}, resulting in high-velocity detonations, the wave speed begins to exceed that of a CJ detonation. This phenomenon is speculated to be a result of reactions occurring within the shock itself, as discussed below.

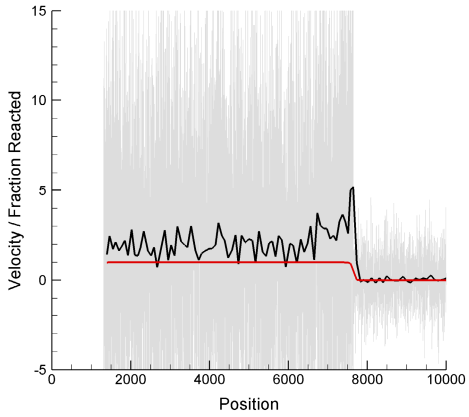


Figure 6. Snapshot of a simulation with a piston of velocity V_{piston} = 2 being driven into a chain of reactive particles previously allowed to come into equilibrium. Grey curve shows each particle velocity, black and red is velocity and reacted fraction averaged over 100 particles.

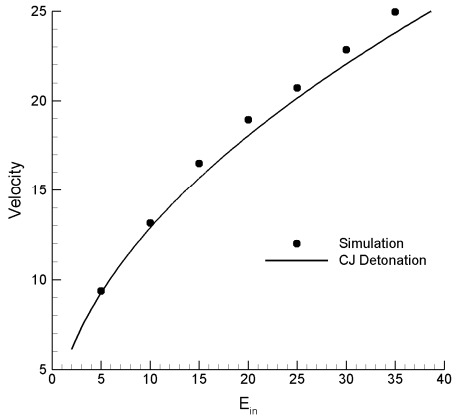


Figure 7. Velocity of detonation in a chain of reactive particles versus energy input, with symbols being the results of simulations and the solid curve being the predictions of Chapman-Jouguet relations.

When the steric factor p was increased toward unity, the value of detonation velocity increased slightly above the CJ value (Fig. 8). For simulations with the steric factor approaching unity, significant reactions occur within the shock front relaxation zone itself, and a weak, rather than Chapman Jouguet, detonation is obtained. This phenomenon had previously been observed in Monte Carlo simulations of detonation with "ultrafast" chemistry by Anderson and Long.[10]

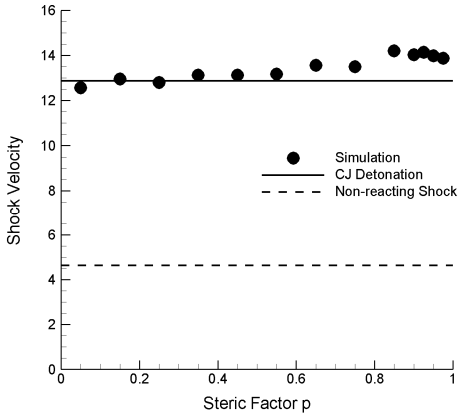


Figure 8. Velocity of detonation in a chain of reactive particles versus steric factor, compared to predictions of Chapman-Jouguet detonation and non-reacting shock.

6 Conclusions

By examining a one-dimensional chain of elastic particles, an exact correspondence between molecular dynamic simulations and the continuum-based treatments for Arrhenius kinetics, Rankine-Hugoniot relations, and Chapman-Jouguet detonations has been demonstrated. The key ingredient beyond the traditional "beads on a wire" model is the use of two alternating masses of particles, rather than just a single particle mass. Only in the case of very fast reactions (steric factor set near unity) are deviations from the Chapman-Jouguet relations observed, which is attributed to weak detonations being realized via ultrafast reactions occurring within the shock front itself.

The use of two-mass systems appears to be a promising candidate for a system that can be "dialed" from classical behavior to non-classical behavior simply by varying the ratio of the particle masses. This study lays the foundation for future forays into systems in which the classical Rankine-Hugoniot relations breakdown. For example, a lattice consisting of uniform masses connected with nonlinear springs supports shock-like waves under piston loading, however, these waves do not agree with the predictions of the Rankine-Hugoniot relations, due to the lack of thermalization (related to the so-called "Fermi-Pasta-Ulam paradox"), and instead the shock-like front is dominated by localized oscillations that can be shown to be solitons. In the case of a highly nonlinear interaction potential it is no longer possible to even define a linear sound speed, giving rise to the concept of "sonic vacuum."[11] Shock waves and detonations is such systems continue to challenge the classical treatments of these phenomena.

Acknowledgements

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