Molecular dynamics simulation of nonlinear waves in granular media

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Abstract—Discrete dynamic equations of spheres in granular chains have been developed so as to simulate the evolution of acoustic signals in these media. The model was built based on Hertzian laws as well as the dissipation effect within the system, and the contact dynamics involving both compression and separation between spheres was also modelled. A molecular dynamics simulation method using the Velocity Verlet algorithm was developed to solve the equations. The strongly nonlinear solitary wave impulses are predicted by the numerical calculations and match the experimental results well. The simulation system has been used as a design tool to determine the optimal chain structure in term of the bandwidth and frequencies which are required within the output impulses. The results exhibit great potential in biomedical applications.

Keywords—granular chain; Velocity Verlet algorithm; nonlinear waves

I. INTRODUCTION

One-dimensional chains of spheres have been investigated and exhibit strongly nonlinear waves, due to nonlinearity of Hertzian interactions between neighboring particles as well as the absence of tensile forces between them in granular media [1-2]. The wave transmission is tunable if a static pre-compression is applied on the chain. The propagation regime can be classified as linear, weakly nonlinear or highly nonlinear, depending on the ratio of the applied dynamic force to the static pre-compression [3]. The concept of a "Sonic Vacuum" was proposed by Nesterenko [2] in "weakly-compressed" granular chains, as classical linear waves cannot propagate through them. However, families of solitary waves as a highly nonlinear mode can be present in such chains. The "Sonic Vacuum" equation is derived based on the continuum model and long-wavelength approximation, and is more general than the KdV wave equation, although the latter is well-known as a basic wave equation for nonlinear problems in many types of material [2]. Solitary waves have been observed in experimental investigations where the applied impulsive signals were generated by mechanical impact of a striker [1-3]. In order to generate solitary wave impulses with a broad bandwidth at higher frequencies within granular media, a different generation method is needed.

In recent years, transient signals from piezoelectric actuators have been used to generate impulses within chains of spheres, and a nonlinear acoustic lens with a tunable focus was created using a two-dimensional array of spherical chains interfaced with water [4]. However, the theoretical analysis and technical details were not presented in [4] to describe the propagation of acoustic wave along the spherical chain with the input of the piezoelectric actuator. Recently our research group has developed a new experimental method, i.e. using high amplitude, narrow bandwidth ultrasonic inputs to produce solitary wave impulses in a single chain of spheres [5]. It has been observed that the travelling waves with in-phase nonlinear normal modes (NNM) can be created in a certain length chain once the excitation amplitude attains a specified threshold value. A controllable frequency band can be realized by designing different chain structures. These new findings exhibit different characteristics from the traditional solitary waves studied in granular media, so it is essential to study the dynamic behaviour of particles in granular chains using resonance excitation. Although the stationary solution of the wave equation reveals the existence of solitary wave in chains of spheres, it cannot explain the periodicity behaviour of the output impulses observed in our experimental system. This is for two reasons. Firstly, the solitary wave is assumed to propagate in an infinite-length chain and it will take infinite-time to return, so the reflection of wave in finite-length chains will not exhibited in the analytical solution in such a model. Secondly, friction and viscoelastic dissipation are not taken into account in the original dynamic equations of particles from which the "Sonic Vacuum" wave equation was derived [2]; thus, the model cannot describe the experimental results accurately, since the dissipation was found to be a very important factor in the generation of the solitary wave impulses observed in our experiments.

Accordingly, in this paper we will develop a novel numerical algorithm to solve the discrete dynamic equations of particles in finite length chains, in which the dissipation effect is also modelled. Given that simulation using a molecular dynamics approach provides the methodology to solve the classical N-body problem effectively [6], we will develop a Velocity Verlet Algorithm to simulate the propagation of acoustic wave along granular chains and reveal the strongly nonlinear behaviour in a resonant particle chain.

II. DYNAMIC MODEL OF PARTICLES IN CHAINS OF SPHERES

First, we will introduce a model to describe the dynamic behavior of particles within finite-length chains, which can resonate. As shown in Fig.1, the spheres in the chain are assumed to have a constant radius R, and are made of the same material. The first sphere is excited by an acoustic transducer, and the last sphere contacts a fixed end. In both cases, the chain contacts a planar surface. Acoustic wave evolution in the granular medium mainly depends on the contact dynamics between particles, but is also affected by the boundary conditions. It assumes that the contact deformation between particles is within the elastic range, so the relationship between the contact force and deformation of the interaction spherical particles can be described by the non-linear Hertzian law [2]. Accordingly, discrete dynamic equations for motion of each sphere in a chain can be constructed, as described in [5].

For the first sphere, the dynamics equation of motion:

$$m\frac{d^2u_1}{dt^2} = \frac{2\sqrt{R}}{3}\left[2\theta_l(\delta_{0l} + u_0 - u_1)^{3/2} - \frac{\theta_m}{\sqrt{2}}(\delta_0 + u_1 - u_2)^{3/2}\right] + \lambda\left(\frac{du_0}{dt} - \frac{du_1}{dt}\right)H(\delta_{0l} + u_0 - u_1) - \lambda\left(\frac{du_1}{dt} - \frac{du_2}{dt}\right)H(\delta_0 + u_1 - u_2) \quad \text{(1-a)}$$

For the second sphere to the penultimate one, the dynamics equation of motion:

$$m\frac{d^2u_i}{dt^2} = \frac{\sqrt{2R}}{3}\theta_m\left[(\delta_0+u_{i-1} - u_i)^{3/2} - (\delta_0 + u_i - u_{i+1})^{3/2}\right] + \lambda\left(\frac{du_{i-1}}{dt} - \frac{du_i}{dt}\right)H(\delta_0 + u_{i-1} - u_i) - \lambda\left(\frac{du_i}{dt} - \frac{du_{i+1}}{dt}\right)H(\delta_0 + u_i - u_{i+1}) \quad \text{(1-b)}$$

For the last sphere, the dynamics equation of motion:

$$m\frac{d^2u_N}{dt^2} = \frac{2\sqrt{R}}{3}\left[\frac{\theta_m}{\sqrt{2}}(\delta_0 + u_{N-1} - u_N)^{3/2} - 2\theta_r(\delta_{0r} + u_N)^{3/2}\right] + \lambda\left(\frac{du_{N-1}}{dt} - \frac{du_N}{dt}\right)H(\delta_0 + u_{N-1} - u_N) - \lambda\frac{du_N}{dt}H(\delta_{0r} + u_N) \quad \text{(1-c)}$$

In Eq. 1, $u_1, u_2, u_3, \dots, u_n$ are the displacements of the center of spheres under the input displacement u_0 from the boundary, and m is the mass of each sphere. The linear damping coefficient λ is used to model the inherent dissipation of the particles as they vibrate within a resonant chain. The damping force is in effect when the spheres are in contact, so the Heaviside function H on the relative displacement of spheres is incorporated into the equations [7]. The material property-related values are given by equations:

$$\frac{1}{\theta_l} = \frac{1-\nu_l^2}{E_l} + \frac{1-\nu_s^2}{E_s} \quad \theta_m = \frac{E_s}{1-\nu_s^2} \quad \frac{1}{\theta_r} = \frac{1-\nu_r^2}{E_r} + \frac{1-\nu_s^2}{E_s} \quad (2)$$

where E_s and ν_s are the Young's modulus and Poisson ratio of spheres; E_l and ν_l are that of the left transducer, and E_r and ν_r are that of the right fixed end. The initially relative displacements under the static force F_0 are given by

$$\delta_{0l} = \left(\frac{3F_0}{4\sqrt{R}\theta_l}\right)^{2/3} \quad \delta_0 = \left(\frac{3F_0}{\sqrt{2R}\theta_m}\right)^{2/3} \quad \delta_{0r} = \left(\frac{3F_0}{4\sqrt{R}\theta_r}\right)^{2/3} \quad (3)$$

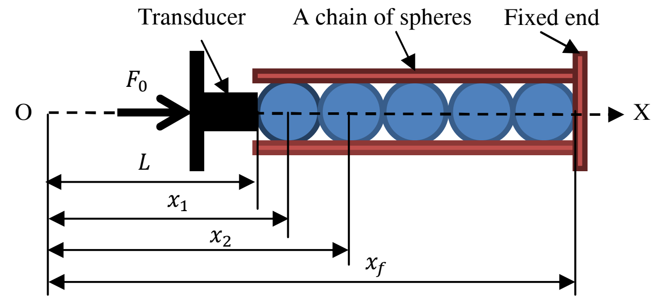

Fig. 1. Illustration of generation of an acoustic propagation in finite-length chains of spheres.

III. A VELOCITY VERLET ALGORITHM OF SOLVING DISCRETE DYNAMIC EQUATIONS OF PARTICLES

Molecular dynamics simulation is an effective numerical tool to calculate how positions, velocities, and orientations of particles in chains change over time. The integration algorithm is based on the basic relationships between force, acceleration, velocity and position as follows:

$$\vec{F_i} = m_i\vec{a}_i \quad \vec{a}_i = {d\vec{v}_i}/{dt} \quad \vec{v}_i = {d\vec{r}_i}/{dt} \quad (4)$$

The Velocity Verlet algorithm is a generally used integrator which has improved accuracy compared to the standard Verlet algorithm [6], since it is derived from expansions of both position and velocity. In order to solve Eq. (1), a numerical method based on Velocity Verlet algorithm has been developed. Here, x_i^j, v_i^j, a_i^j and F_i^j are used to represent position, velocity, acceleration and the force acting on the i[th] sphere respectively in the transmission of a wave in a chain of N spheres at time $j\delta t$. δt is time step, i and j are the order of spheres in the chain and time count respectively. Here, $i = 1, 2, \cdots N$, and N_t is the maximum time count, where $j = 0, 1, 2, \cdots, N_t$.

In the first step, the initial positions of the spheres (x_i^0) and the transducer needs to be determined. This work starts from the last sphere since it is assumed to contact with the fixed end. As shown in Fig.1, the position of the contact point between the last sphere and the fixed end is assumed to be $x_f = L + 2RN$. Then, the initial positions of the spheres are calculated one by one from this end, using the relative displacements which are given in Eq. (3), until the position of the first sphere as well as that of the front wall of the actuating transducer (x_0^j) are determined.

In the second step, a time loop is established so as to solve Eq. (1), using the Velocity Verlet algorithm. This proceeds in a logical sequence. At each integration cycle, the algorithm evaluates the motion of each sphere in the following order (steps A-D):

A. Calculate the particle velocities of the spheres at time-step $j+\frac{1}{2}$:

$$v_i^{j+\frac{1}{2}} = v_i^j + \frac{1}{2}a_i^j \delta t$$

B. Calculate positions of the spheres at time-step $j+1$:

$$x_i^{j+1} = x_i^j + v_i^{j+\frac{1}{2}}\delta t$$

C. Calculate the acting forces and accelerations of the spheres at time-step $j+1$:

For the first sphere:

$$\delta_{0l} + u_0^{j+1} - u_1^{j+1} = R - (x_1^{j+1} - x_0^{j+1}),$$

where, if $(R - (x_1^{j+1} - x_0^{j+1})) < 0$ (*i.e.* separation between the first sphere and the transducer appears), then:

$\delta_{0l} + u_0^{j+1} - u_1^{j+1} = 0$, and $F_{10}^{j+1} = 0$; otherwise

$$F_{10}^{j+1} = \frac{4\theta_l\sqrt{R}}{3}(R - (x_1^{j+1} - x_0^{j+1}))^{3/2} + \lambda(v_0^{j+\frac{1}{2}} - v_1^{j+\frac{1}{2}})$$

$$\delta_0 + u_1^{j+1} - u_2^{j+1} = 2R - (x_2^{j+1} - x_1^{j+1}).$$

Also, if $(2R - (x_2^{j+1} - x_1^{j+1})) < 0$ (*i.e.* separation between the first and the second sphere occurs), then:

$\delta_0 + u_1^{j+1} - u_2^{j+1} = 0$ and $F_{12}^{j+1} = 0$; otherwise

$$F_{12}^{j+1} = \frac{\sqrt{2R}\theta_m}{3}(2R - (x_2^{j+1} - x_1^{j+1}))^{3/2} + \lambda(v_1^{j+\frac{1}{2}} - v_2^{j+\frac{1}{2}})$$

$F_1^{j+1} = F_{10}^{j+1} - F_{12}^{j+1}$ and $a_1^{j+1} = F_1^{j+1}/m$

For the second sphere to the penultimate one:

$$\delta_0 + u_{i-1}^{j+1} - u_i^{j+1} = 2R - (x_i^{j+1} - x_{i-1}^{j+1}),$$

where, if $(2R - (x_i^{j+1} - x_{i-1}^{j+1})) < 0$ (*i.e.* separation between the ith sphere and its left sphere appears), then:

$\delta_0 + u_{i-1}^{j+1} - u_i^{j+1} = 0$ and $F_{i(i-1)}^{j+1} = 0$; otherwise

$$F_{i(i-1)}^{j+1} = \frac{\sqrt{2R}\theta_m}{3}(2R - (x_i^{j+1} - x_{i-1}^{j+1}))^{3/2} + \lambda(v_{i-1}^{j+\frac{1}{2}} - v_i^{j+\frac{1}{2}})$$

$$\delta_0 + u_i^{j+1} - u_{i+1}^{j+1} = 2R - (x_{i+1}^{j+1} - x_i^{j+1}).$$

Also, if $(2R - (x_{i+1}^{j+1} - x_i^{j+1})) < 0$ (*i.e.* separation between the ith sphere and its right sphere appears), then:

$\delta_0 + u_i^{j+1} - u_{i+1}^{j+1} = 0$ and $F_{i(i+1)}^{j+1} = 0$; otherwise

$$F_{i(i+1)}^{j+1} = \frac{\sqrt{2R}\theta_m}{3}(2R - (x_{i+1}^{j+1} - x_i^{j+1}))^{3/2} + \lambda(v_i^{j+\frac{1}{2}} - v_{i+1}^{j+\frac{1}{2}})$$

$F_i^{j+1} = F_{i(i-1)}^{j+1} - F_{i(i+1)}^{j+1}$ and $a_i^{j+1} = F_i^{j+1}/m$

Finally, for the last sphere:

$$\delta_0 + u_{N-1}^{j+1} - u_N^{j+1} = 2R - (x_N^{j+1} - x_{N-1}^{j+1}),$$

where if $(2R - (x_N^{j+1} - x_{N-1}^{j+1})) < 0$ (*i.e.* separation between the last sphere and the penultimate one appears), then

$\delta_0 + u_{N-1}^{j+1} - u_N^{j+1} = 0$ and $F_{N(N-1)}^{j+1} = 0$; otherwise

$$F_{N(N-1)}^{j+1} = \frac{\sqrt{2R}\theta_m}{3}(2R - (x_N^{j+1} - x_{N-1}^{j+1}))^{3/2} + \lambda(v_{N-1}^{j+\frac{1}{2}} - v_N^{j+\frac{1}{2}})$$

$$\delta_{0r} + u_N^{j+1} = R - (x_f - x_N^{j+1})$$

Also, if $R - (x_f - x_N^{j+1}) < 0$ (*i.e.* separation between the last sphere and the fixed end appears), then:

$\delta_{0r} + u_N^{j+1} = 0$ and $F_{Nf}^{j+1} = 0$; otherwise

$$F_{Nf}^{j+1} = \frac{4\theta_r\sqrt{R}}{3}(R - (x_f - x_N^{j+1}))^{3/2} + \lambda v_N^{j+\frac{1}{2}}$$

$F_N^{j+1} = F_{N(N-1)}^{j+1} - F_{Nf}^{j+1}$ and $a_N^{j+1} = F_N^{j+1}/m$

D. Update the particle velocities of the spheres:

$$v_i^{j+1} = v_i^{j+\frac{1}{2}} + \frac{1}{2}a_i^{j+1}\delta t$$

E. Update Time and Repeat A-D Steps.

Based on the above algorithm, a C++ program was developed to solve the position, particle velocity and acceleration of individual particles at a time while the chain is excited, and hence the acoustic propagation can also be simulated.

IV. ANALYSIS OF SIMUALTION RESULTS

Using the developed simulation tool, we will present two examples of the predicted results. Firstly, we will simulate the propagation of ultrasonic signals in a chain using a sinusoidal tone-burst input of finite duration and constant amplitude; in addition, we will directly use the measured input waveform that we have used in actual experiments to predict the resultant impulses. As shown in Fig.1, we assume that the spheres are made of chrome steel, and the properties of the spheres are: R=0.5 mm; E_s = 201 GPa; ν_s = 0.3 and the density is ρ_s = 7833 Kg/m^3. The material parameters for the actuating transducer (to the left of Fig. 1) are E_l = 201 GPa and ν_l = 0.3, and for the fixed end (at the right) are E_r = 2.45 GPa and ν_r = 0.35 (acrylic polymer). λ = 0.32 Nsm^{-1} is used. In addition, a static pre-compression force of the order of 0.01 N is assumed to exist in the chain to generate the solitary wave impulses.

A. Simulation of the propagation of the ultrasonic signal

For a finite-length chain containing 6 spheres, a sinusoidal tone-burst containing 20-cycles at 73 kHz is used as the input signal, with the displacement amplitude of the input being 1.0 μm . δt =10^{-8} s is used. The velocity waveform and the spectrum of the first sphere, the fourth sphere and the last sphere are illustrated in Fig. 2 and Fig. 3 respectively. As seen in Fig. 2, the solitary wave impulses can be generated under such an input condition and chain construction. The propagation of the solitary wave is represented by the red arrow, and the transmission of the wave reflected from the right-hand wall is indicated by the blue arrow. Due to the action of the excitation and the reflected wave, solitary wave impulses with a characteristic period are formed, and the nonlinear normal mode (NNM) that results is characterized by the appearance of both harmonics and sub-harmonics of the input frequency, as shown in Fig. 3. The waveform of the last sphere has a longer time duration, and accordingly a narrower frequency bandwidth. This can be attributed to the fact that the reflected wall is made of a softer material (acrylic polymer) with respect to the steel spheres, which results in higher percentage of sub-harmonic content in the output impulses present at the last sphere.

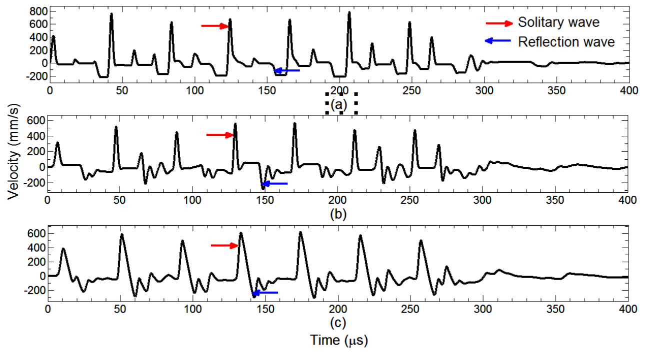

Fig. 2. Simulation of the propogation of a nonlinear wave in a 6-sphere chain, showing particle velocity waveforms for (a) the first sphere, (b) the fourth sphere and (c) the last sphere.

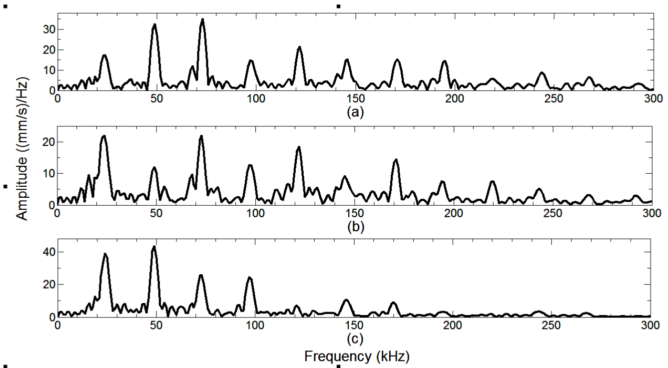

Fig. 3. Spectrum of the particle velocity waveforms shown in Fig. 2, for (a) the first sphere; (b) the fourth sphere and (c) the last sphere.

B. *Simulations to compare to experimental results*

In addition, we simulate the ultrasound evolution based on the experimental conditions outlined in [5]. The first sphere was excited harmonically by a longitudinal ultrasonic horn at 73 kHz and a tone-burst length of 45 cycles was used. In the experiments, the last sphere was positioned against an acrylic aperture, so that the particle velocity signal of the ultrasonic horn and that of the last sphere in the chain were both recorded using a laser vibrometer, and are referred to as the input and output signals of the granular chain. Both the measured velocity waveform of the horn and the corresponding displacement by integration are used as input signals in the simulation to calculate the signals that would be output by the last sphere. Note that, experimentally, the output from the horn was not a tone-burst of constant amplitude, but had a longer rise and fall time, as well as an increased time duration, as the input voltage was increased.

In order to observe experimentally the evolution of the ultrasonic wave along the chain with an increase of the input amplitude, the output of the horn was increased, and three velocity waveforms (at peak-peak maximum particle velocity amplitudes of 675 mm/s, 864 mm/s and 1081 mm/s respectively) were recorded in experiments. These were then used as an input for the simulation. The simulation results are shown in Fig. 4. With the increase of the input particle velocity amplitude, the resultant waveform of the last sphere gradually changes from a weakly non-linear to a strongly non-linear behavior, and the solitary wave impulses are generated once the input signals rises above a specific threshold value. The results presented in Fig. 4 are also observed in our experimental results [5] to which they correspond well.

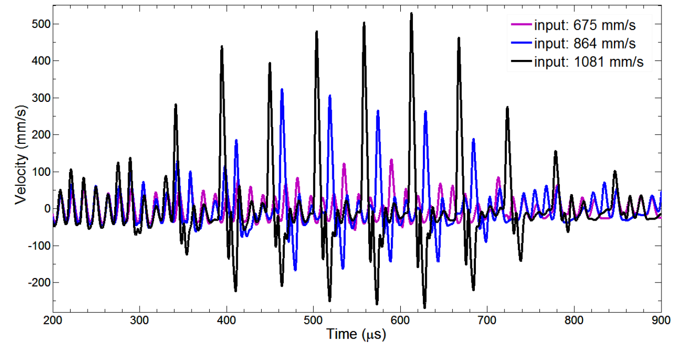

Fig. 4. Simulation of the particle velocity waveforms of the last sphere, using selected pk-pk particle velocity input amplitudes. The evolution of solitary wave impulses is clearly seen.

V. Conclusions

In order to simulate acoustic wave propagation in granular chains, a mathematical model has been used to describe the dynamics of particles in a chain of finite length. A Velocity Verlet Algorithm has been developed to solve the equations of an N-sphere system. This method provides a highly-effective tool to study the propagation of nonlinear wave, and the generation of solitary wave impulses.

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