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The dynamic excitation of a granular chain for biomedical ultrasound applications: contact mechanics finite element analysis and validation

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Abstract. There has been recent interest in the transmission of acoustic signals along granular chains of spherical beads to produce waveforms of relevance to biomedical ultrasound applications. Hertzian contact between adjacent beads can introduce different harmonic content into the signal as it propagates. This transduction mechanism has the potential to be of use in both diagnostic and therapeutic ultrasound applications, and is the object of the study presented here. Although discrete dynamics models of this behaviour exist, a more comprehensive solution must be sought if changes in shape and deformation of individual beads are to be considered. Thus, the finite element method was used to investigate the dynamics of a granular chain of six, 1 mm diameter chrome steel spherical beads excited at one end using a sinusoidal displacement signal at 73 kHz. Output from this model was compared with the solution provided by the discrete dynamics model, and good overall agreement obtained. In addition, it was able to resolve the complex dynamics of the granular chain, including the multiple collisions which occur. It was demonstrated that under dynamic excitation conditions, the inability of discrete mechanics models to account for elastic deformation of the beads when these lose contact, could lead to discrepancies with experimental observations.

1. Background

Granular chains are usually defined as one-dimensional alignments of generally spherical particles. The interactions between such particles are governed by the laws of contact mechanics. The study of granular chains is of interest to a range of disciplines in science and engineering. Granular chains have been relevant to applications where they can serve as a type of waveguide and/or information carrier by transmitting, redirecting, or blocking solitary waves in a controllable and efficient manner [1]. Solitary waves haves been known to be generated in a one-dimensional granular chain of spherical particles, where dispersive and nonlinear effects, due to the discreteness of the system and the Hertzian contact among spheres balance out [2], [3], [4]. Through the use of a discrete mechanics

model, solitary waves were first shown to be supported in a granular chain by Nesterenko in 1983 [2]. This theoretical observation was subsequently confirmed experimentally by Lazaridi and Nesterenko in 1985 [5]. Coste *et al* [6] carried out an experimental studied of the propagation of high-amplitude compressional waves in a chain of beads in Hertzian contact, submitted or not to a small pre-compressional static force. An extensive range of pulse amplitudes was investigated, and it was concluded that the shape and velocity the solitary waves as functions of their maximum amplitude were in good agreement with results from the discrete mechanics model.

Interest in the generation of solitary waves in a granular chain has recently been extended to biomedical applications [7], [8]. In [7], the generation of high-amplitude focused acoustic pulses using a one-dimensional array of granular chains was investigated, where the amplitude, size, and location of the focus could be controlled by varying the static pre-compression of the chains. Such an array could have important applications to both therapeutic high-intensity focused ultrasound applications and also perhaps in imaging. It is however yet unclear which advantages a transduction mechanism based on the non-linear dynamics of granular chains may have compared with more commonly used arrays of piezoelectric transducers, such as those described in [9]. Furthermore, the dimensions of the array as well as the frequencies involved in the configuration described in [7] are not in fact pertinent to biomedical ultrasound. Hence, further studies are clearly required, which involve excitation protocols which are relevant to clinical ultrasound applications.

In [8], large amplitude displacements were produced by a resonant 73 kHz ultrasonic source to drive a granular chain consisting of six 1 mm diameter chrome steel beads. Travelling solitary wave impulses were observed, which were due to both non-linearity between adjacent spheres and reflections within the chain. The resulting impulses in the axial velocity measured at the final bead of the chain were found to possess both high amplitude and wide bandwidth, featuring spectral content up to 200 kHz. These distinctive features suggest that such signals could be harnessed for both therapeutic and diagnostic ultrasound applications.

In [8], predictions of the bead dynamics based on the discrete mechanics model proposed by Lydon *et al* [10] reproduced characteristics of the laser vibrometer measurements of the velocity of the final bead of the granular chain. This observation, together with the comparisons in [5], [6] and [10] suggest that discrete mechanics models clearly replicate salient features of experimental observations. Nevertheless, to better understand and optimise the transduction process and make it application-specific, it is desirable to move beyond discrete mechanics formulations. Indeed, a transducer for biomedical ultrasound applications comprising a granular chain may include other components, such as piezoelectric actuator and matching layers. Furthermore, the transducer will couple into an acoustic medium, such as water or soft tissue, the loading of which will affect its dynamic behaviour. Hence, a numerical solution to the design of such a transducer is likely to provide more flexibility in designing an application-specific device.

Finite element analysis (FEA) is routinely used to solve contact mechanics problems in engineering [11]. Many commercially available FEA packages also allow for electro-mechanical coupling with piezoelectric elements, as well as fluid-structure coupling, and can therefore predict the radiated acoustic pressure for a known input voltage. Musson and Carlson [12] proposed an FEA of the non-linear dynamics of the granular chain investigated by Lazaradi and Nesterenko [5]. They demonstrated that solitary waves can be generated in a chain of 20 beads using FEA. This solution was provided by the COMSOL Multiphysics software [13], and the analysis demonstrated the importance of localised plastic deformations in the dynamics of granular chains. In discrete mechanics models, these plastic deformations are neglected, as the beads are assumed to be point masses [6].

The excitation of the first bead of the chain considered in [12] was of the same type as that was assumed in [5] and consisted of a single constant velocity impact. Whilst it is encouraging that the FEA generated improved agreement with the experimental work in [5] relative to the discrete mechanics model, further work is clearly required to extend this type of analysis to excitation signals of relevance to biomedical ultrasound. It is therefore of interest to investigate whether FEA can successfully predict the response of a granular chain to the high-amplitude and high-frequency

excitation signals described in [8]. The work described in this paper constitutes a preliminary investigation where it was initially verified that Hertz' contact law [14] was satisfied for two spheres undergoing static compression. Subsequently, the six-bead granular chain described in [8] was excited with five cycles of a sinusoidal displacement, via a rigidly vibrating cylindrical piston. The amplitude of the displacement excitation was 0.3 μm. The frequency of excitation was also the same as the fundamental frequency of the excitation waveform used in [8], i.e. 73 kHz. The FEA was carried out using a transient analysis in ANSYS Mechanical version 15.0 [14]. Displacements at the centre of each bead were obtained as a function of time and compared with results from the discrete mechanics model described in [10], as implemented in [8], and in absence of any viscous damping. The FEA results were in good overall agreement with the discrete mechanics model. To investigate the source of the discrepancies between both models, the elastic deformations of the beads along the axis of the chain were analysed, as a function of time.

2. Theory

When the surfaces of two separate bodies touch each other so that they become mutually tangential, they are said to be in contact. In the physical sense, the surfaces that are in contact do not interpenetrate and can transmit compressive normal forces and tangential frictional forces. They do not generally transmit tensile normal forces and are thus free to separate and move away from each other.

The static frictionless interaction between two adjacent elastic spheres is an exact solution of linear elasticity and is known as Hertz's law [14]. As a result of geometrical effects, there exists a nonlinear relationship between the exerted force F_0 on the spheres and the distance of approach δ_0 of their centers. For homogeneous isotropic spheres of radius a, this is expressed as follows [6]:

$$\delta_0 = \frac{2(\theta F_0)^{2/3}}{a^{1/3}} \tag{1}$$

where

$$\theta = \frac{3(1-v^2)}{4E} \tag{2}$$

where E and v are respectively Young's modulus and Poisson's ratio corresponding to sphere material.

In the case of a dynamic excitation, this solution is expected to remain valid when the applied force and hence the distance of approach are both slowly varying functions of time [6]. According to [6], the variations may be considered as slow if every typical time scale involved in the motion is much greater than the time needed by a bulk longitudinal acoustic wave to travel across the diameter of a bead. In such cases, a discrete mechanics model has been proposed to model a chain of N identical beads, which essentially consists of a one-dimensional system of point masses linked by nonlinear springs. This can be expressed as a system of coupled nonlinear differential equations, where the equation of motion of the ith bead is given by [6]:

$$\ddot{u}_i = \frac{1}{2m\theta}\sqrt{\frac{a}{2}}\left([\delta_0 - (u_i - u_{i-1})]^{3/2} - [\delta_0 - (u_{i+1} - u_i)]^{3/2}\right) \tag{3}$$

where u_i is the displacement at the centre of the ith bead and $\ddot{u}_i$ is its second derivative with respect to time. The mass m associated with each bead is equal to $\frac{4\pi\rho a^3}{3}$, where ρ is the density of the bead material. This formulation neglects dissipation effects which may arise from the beads' viscoelasticity. It also neglects the plastic deformation of the beads. An extension to this model was proposed by Lydon *et al* [10] to address the lack of dissipative effects in equation (3) and to better reflect potential experimental conditions. Indeed, although viscoelastic effects may be small in materials such as steel,

the beads require a holder to keep them axially aligned during excitation. Such a holder is likely to introduce dissipative effects. To account for this, Lydon *et al* [10] introduce a linear viscous damping coefficient between successive spheres in the dynamic equations. The damping term is only relevant when the spheres are in contact and this is controlled by means of a Heaviside function. Loss of contacts between the beads can be accounted for by noting that only positive arguments of the 3⁄2 power-law terms in equation (3) need be considered. These terms can be set to zero for negative values of these arguments, i.e. tensionless behaviour, when the spheres lose contact. This model was used in [8] to simulate the dynamics of a chain of six chrome steel spheres in Hertzian contact. The model also considers contact of the first and last sphere of the chain with spheres of infinite radius, thus approximating walls of a semi-infinite domain. In the investigations carried out in [8] and [10], the first sphere is therefore effectively excited by a flat surface possessing the properties of the ultrasonic horn tip exciting the chain, as the last sphere is in contact with a static wall possessing the properties of the support. These contacts are assumed to be Hertzian in nature.

The work carried out by Hutchins *et al* [8] was used as a starting point for the dynamic analysis described in this paper. The granular chain consists of six spherical chrome steel beads. It was assumed that no pre-compressional static force was acting along the axis of the chain, so that the beads were just touching. Although this situation implies that no acoustic waves can propagate up and down the chain, it is known to lead to highly non-linear behaviour [6], which is more likely to generate signals relevant to biomedical ultrasound [7], [8]. All FEA was carried out using ANSYS™ Mechanical version 15. The beads were assumed to be perfectly aligned, so that an axisymmetric analysis could be opted for, whereby the Cartesian y-axis defined the axis of symmetry of the granular chain, and the analysis was carried out in the x-y plane. The first bead of the chain was excited via a cylindrical piston whose degrees of freedom were coupled to ensure rigid body motion. A rigidly vibrating piston was employed to reduce uncertainties when comparing with the discrete mechanics model in [8] and [10], since modelling semi-infinite structures using FEA presents challenges. For similar reasons, the final bead of the chain was assumed to be in contact with a rigid support. All contacts were assumed to be frictionless, thus simulating Hertzian contacts. The introduction of a linear viscous damping coefficient between successive spheres, as proposed in [10], was not implemented as part of this work. Again, including this type of damping in the FEA model would add a layer of complexity to the validation process. Hence, dissipative mechanisms will be neglected here and dealt with in a separate paper.

It is common to formulate the problem of frictionless contact between two solid bodies as a variational inequality. This presents a special type of minimisation problem with inequality constraints, which can be efficiently treated in a standard manner, i.e. with (1) the penalty method, (2) the augmented Lagrangian method or (3) the Lagrange multiplier method [11]. The ANSYS™ Mechanical v15.0 FEA package includes these three options as formulations to establish a relationship between two surfaces to prevent or limit them from passing through each other during the analysis. For an in-depth description of these methods, the reader is referred to Chapter 4 of [11]. Methods (1) and (2) are both penalty-based and invoke the concept of contact stiffness i.e. the virtual work due to the deformation of imaginary springs at the contact interface term. This inevitably results in some degree of penetration between the two surfaces, depending on the chosen value for the contact stiffness term. Method (3), or the Normal Lagrange Formulation as it is described in ANSYS Mechanical, adds an extra degree of freedom (contact pressure) to satisfy contact compatibility. Consequently, instead of resolving contact force as contact stiffness and penetration, contact pressure is solved for explicitly as an extra degree of freedom. This has the advantage of enforcing near-zero penetration when modelling frictionless contact between two bodies. This formulation however requires the use of a direct rather than an iterative solver, which may limit the size of the models solved due to larger RAM requirements. Fortunately, the geometry of granular chain could be defined using an axisymmetric coordinate system. Hence, computational requirements were not an impeding factor.

Given the complexity of the dynamics of the six-bead granular chain under the excitation conditions described in [8], it is likely that any effects of penetration between two adjacent surfaces will lead to uncertainties in the displacements of the beads that will propagate throughout the system as time increases. This will constitute a source of disagreement between the FEA and the discrete mechanics model. For this reason, the Normal Lagrange Formulation was opted for over the penalty and augmented Lagrangian formulations.

3. Results

Prior to carrying out a dynamic FEA of the six-bead granular chain described in Section 2, the case of the static compression of two 1 mm diameter chrome steel spheres was investigated so as to determine to which extent Hertz' contact law was satisfied. The configuration was assumed to be axisymmetric, the Cartesian y-axis being the axis of symmetry. The top-most sphere was stressed by a static force, applied in the negative y-direction, as shown in figure 1. The bottom-most sphere was assumed to be in Hertzian contact with a rigid support. The region of contact common to both spheres was also assumed to be Hertzian. The applied force was varied between 0.5 N and 5 N. The material properties of the sphere material were the same as those assumed by Hutchins *et al* (2015), i.e.:

- Young's modulus: 201 GPa;
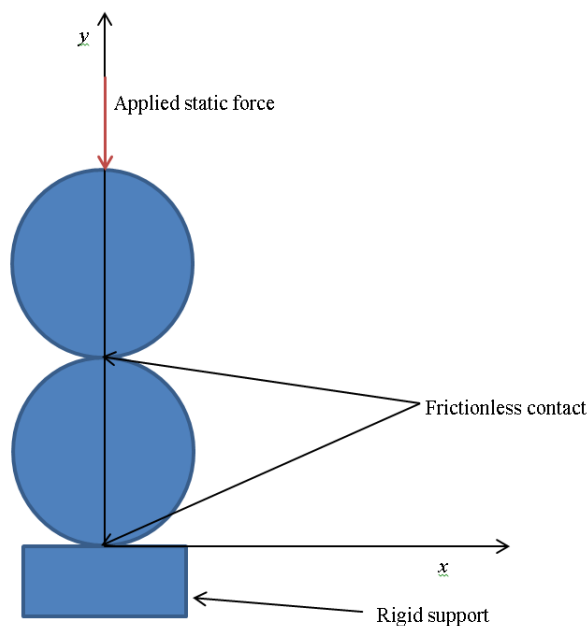- Density: 7833 kg m^{-3};
- Poisson's ratio: 0.3.

Figure 1. Schematic diagram of two-sphere configuration.

Particular attention was given to the mesh density around the contact regions. Indeed, contact mechanics problems in FEA tend to require mesh refinements around such regions [12], [15]. A close-up view of the mesh around the contact between both spheres is shown in figure 2.
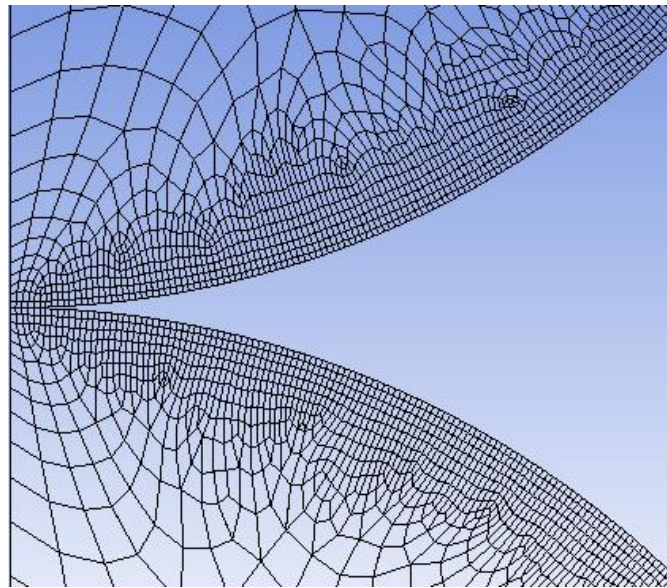
Figure 2. Close-up of mesh around contact region between both spheres.

When two spheres in Hertzian contact each undergo a static force F_0, the distance of approach between the centre of each sphere is given by equation (1) [6]. After post-processing the displacements at the centres of the spheres the y-direction, the distance of approach was calculated and compared with the corresponding analytical solution predicted by equation (1). The distance of approach as a function of the applied static force is shown in figure 3. Both the analytical solution obtained from equation (1), as well as the FEA results are shown.
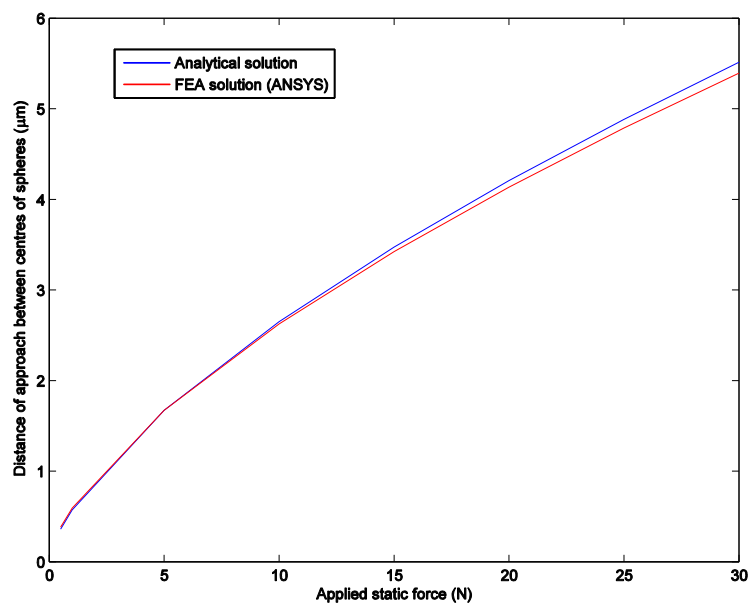
Figure 3. Distance of approach between two spheres in Hertzian contact.

The percentage difference between the analytical solution and the FEA is displayed in figure 4.
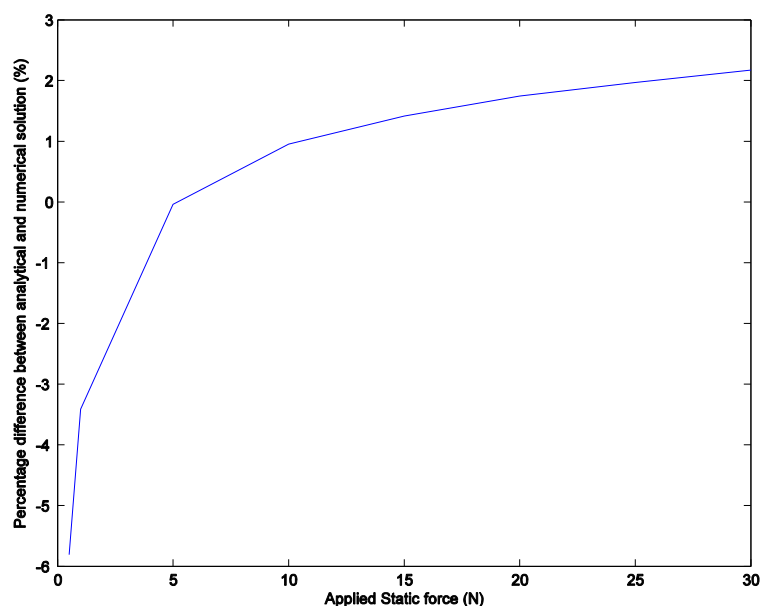
Figure 4. Distance of approach between two spheres in Hertzian contact: percentage difference between analytical solution and FEA.

It can be seen that for this configuration, over the range of applied forces investigated, the agreement between the FEA is within -6% and +2% of the analytical solution. For lower values of the applied force it is likely that issues of numerical tolerance arise, due to the small displacement magnitudes. For larger values of the applied force, an increasingly finer mesh is required around the contact region to minimise the difference between the analytical solution and the FEA. Nevertheless, this level of agreement was considered satisfactory and the case of the dynamic excitation was subsequently investigated.

As described in Section 2, the dynamic excitation case featured a granular chain of six 1 mm diameter chrome steel spheres. The top-most sphere (sphere 1) was excited by a cylindrical piston of 0.2 mm height and of 0.5 mm radius, moving as a rigid body and excited along the *y*-direction by five cycles of a sinusoidal displacement of 0.3 μm magnitude at a frequency of 73 kHz. The final sphere of the chain (sphere 6) was assumed to be in frictionless contact with a rigid support (see figure 5).
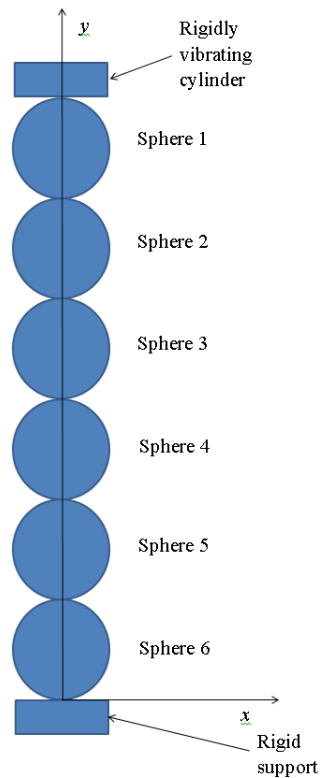
Figure 5. Schematic diagram of six-sphere configuration.

Using a time step of 0.1 μs, a transient analysis was carried out in ANSYS Mechanical, over a time period of 68.5 μs, i.e. for five cycles of the 73 kHz displacement excitation. The Normal Lagrange Formulation was adopted, as described in Section 2. A corresponding discrete mechanics calculation was carried out using the model described in [10], as implemented in [8] and in absence of dissipative effects. The displacement along the y-direction at the centre of each sphere is plotted in figures 6a to 6f, corresponding to spheres 1 to 6, respectively.

6a Sphere 1

6b Sphere 2

6c Sphere 3

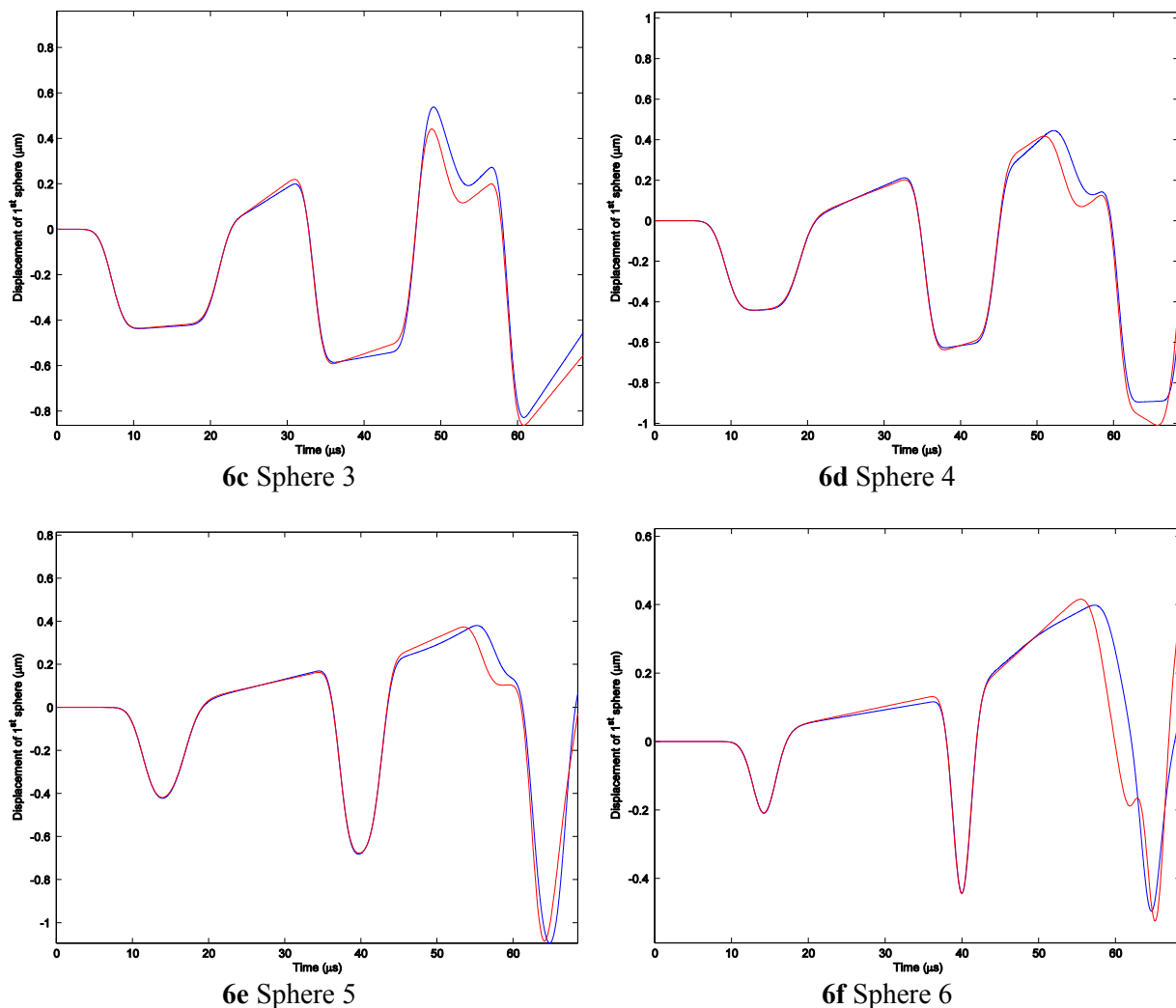**6d** Sphere 4

6e Sphere 5
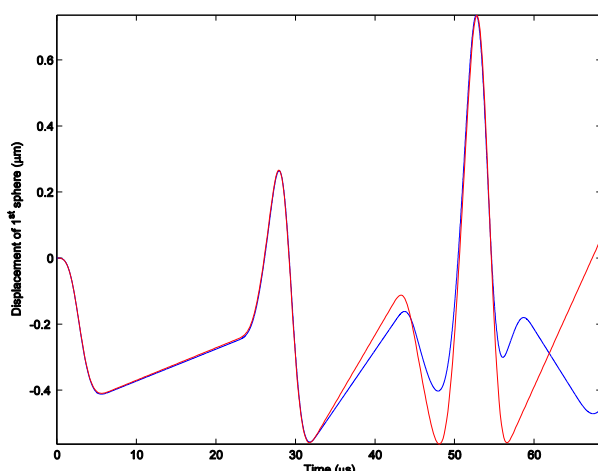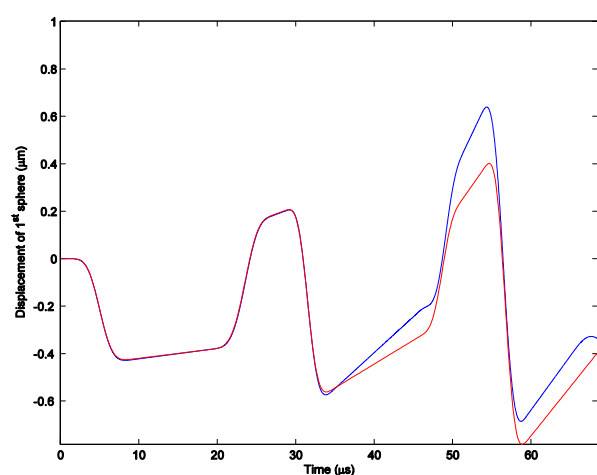
6f Sphere 6

Figure 6 Displacement of the centres of spheres 1 to 6 along the axis of the granular chain as a function of time. The discrete mechanics solution is shown in blue and FEA results are shown in red.

An animation of the total deformation of the beads throughout the five cycles of the 73 kHz displacement excitation can be visualised at the following link: Six-bead granular chain dynamic excitation, where for visualisation purposes, the deformations have been scaled up by a factor of 90.

The above animation clearly shows the wave generated by the impact of the piston on the first bead of the chain. During the excitation cycle, the beads can be seen to lose contact and collide with one another and with the support and the vibrating piston. This effect did not arise in the investigation carried out in [12], due to the nature of the excitation. The impression of penetration of adjacent surfaces in the animation is a result of the large scaling factor. It was verified by post-processing the results that the Normal Lagrange Formulation does indeed preclude penetration at the contact regions.

The graphs in figure 6 show that the output from the discrete mechanics model follows similar trends to the FEA results, in terms of the variation of displacement amplitudes as a function of time. Multiple collisions between the beads are successfully resolved by the FEA. Differences between both models are mainly characterised by time delays in the FEA data, relative to the discrete mechanics waveforms. Indeed, the FEA waveforms appear to lag behind the discrete mechanics results, and it can be seen that the time delay increases as a function of time. Refinement of the numerical solver time step and of the mesh density did not improve the agreement between both models. It is therefore likely that the elastic deformation of the beads is responsible for this. Clearly, if the beads lose contact after

being compressed and do not get the chance to return to their equilibrium spherical shape upon the next impact, this will generate a delay relative to the time of impact estimated using the discrete mechanics model. As successive deformations and impacts occur as the wave propagates up and down the chain, this delay is likely to increase further, and agreement between both models will gradually worsen.

In order to confirm this, the elastic deformation of the beads was investigated. This was done by calculating the cross-sectional distance of each bead along the axis of the granular chain, as a function of time. The result for the first bead is displayed in figure 7.
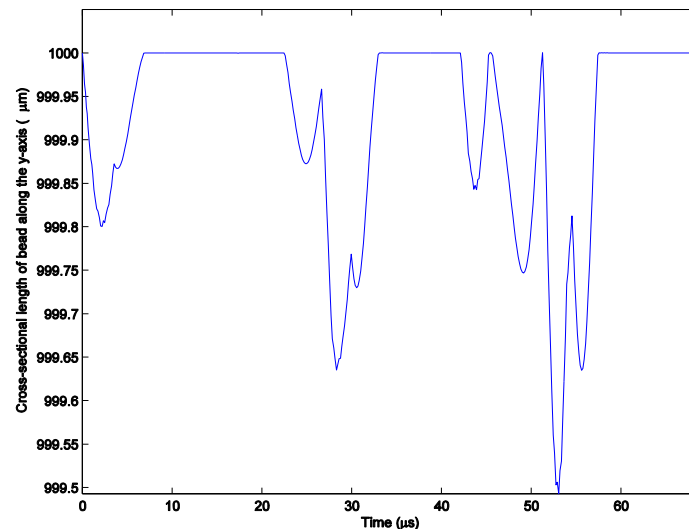

Figure 7 Variation with time of the cross-sectional length of the first bead of the granular chain.

The results in figure 7 clearly show that the bead indeed does not necessarily return to its equilibrium spherical shape upon successive impacts. Additionally, the elastic deformation of the bead can be seen to be of the order of the piston maximum displacement amplitude, which is 0.3 μm. This observation, which is also valid for the other beads of the chain, highlights a limitation of discrete mechanics models when investigating the dynamics of granular chains.

4. Conclusions

This work constitutes a preliminary investigation towards designing novel devices for biomedical ultrasound applications, whose transduction process will rely on non-linear phenomena arising from the dynamic excitation of granular chains.

A finite element model was developed in ANSYS Mechanical to simulate the dynamic behaviour of a granular chain consisting of six spherical beads of 1 mm diameter. The first bead of the chain was excited by a rigidly vibrating cylindrical piston, undergoing a 0.3 μm amplitude sinusoidal displacement, along the direction of the axis of the chain at a frequency of 73 kHz and for five cycles. Initially, it was ensured that Hertz' contact law was satisfied for the static case of two pre-compressed spheres. Subsequently, axial displacements at the bead centres obtained from the FEA of the dynamic excitation of the chain were compared with results from the well-known discrete mechanics model. Good overall agreement between both models was observed. There were, however, discernible differences which were attributed in part to the elastic deformation of the beads, which is not accounted for in the discrete mechanics model when the beads separate.

In [12], it was reported that plastic deformations of the beads could constitute a source of dissipation and lead to differences between experimental data and results from discrete mechanics models. The study reported in this paper investigates the dynamics of a granular chain with excitation

and boundary conditions which cause the beads to separate and collide with one another, which was not the case in [12]. This present study therefore highlights a potential additional source of disagreement between experimental results and discrete mechanics models, in the dynamic analysis of granular chains.

Acknowledgements

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