The dynamic excitation of a granular chain: contact mechanics finite element analysis and experimental validation

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Abstract

There is currently interest in transmitting acoustic signals along granular chains to produce waveforms of relevance to biomedical ultrasound applications. The study of such a transduction mechanism is greatly aided by the use of validated theoretical models. In view of this, a finite element analysis is presented in this paper. The dynamics of a granular chain of six, 1 mm diameter chrome steel spherical beads, was excited at one end using a sinusoidal displacement signal at 73 kHz, and terminated by a rigid support. Output from this model was compared with the solution provided by the equivalent discrete dynamics model, and good agreement obtained. An experimental configuration involving the same chain, but terminated by an annular support made of a liquid photopolymer resin was also simulated and the velocity of the last sphere obtained through simulation was compared with laser vibrometer measurement, with good agreement. This model was then extended whereby the granular chain was coupled to an acoustic medium with the properties of water, via a thin vitreous carbon cylinder. Finite element predictions of the acoustic pressure indicate that, for a 73 kHz excitation frequency, harmonic rich acoustic pulses with harmonic content close to 1 MHz are predicted.

I. INTRODUCTION

Granular crystals can be thought of as ordered aggregates of elastic particles in contact with each other. They are a type of nonlinear periodic phononic structure.[1] Granular crystals display nonlinear characteristics which result from the nonlinear relationship of the force at the contact and the displacement between neighboring element centers (described by Hertzian contact law – a consequence of linear mechanics) and an asymmetric potential which arises between neighboring elements from the inability of granular crystals to support tensile loads.[1] As a consequence of these nonlinearities, there is a negligible linear range for interaction forces between neighboring elements, in the vicinity of zero pre-compression force applied to the chain.[1] This leads to a non-existent linear sound speed in the uncompressed material, resulting in a phenomenon described as a "sonic vacuum". Under such circumstances, the traditional wave equation does not support a characteristic speed of sound[2]. However, granular crystals are known to support a wide array of nonlinear phenomena, including the generation of compact solitary waves.[3,4,5,6,7,8] A comprehensive review of granular crystals, along with the description of the abundance of nonlinear phenomena that these structures support, can be revealed by consulting the works of Theocharis *et al.*[1] and of Nesterenko.[2]

In granular chains, defined here as one-dimensional granular crystals of spherical beads, the generation of solitary waves is supported where dispersive and nonlinear effects balance out.[3,6,9] This phenomenon was first described by Nesterenko in 1983, where a discrete mechanics model was used to demonstrate that the propagation of solitary waves was supported in a granular chain.[3] This observation was later confirmed in 1985 by generating solitary waves in a chain of spherical beads via the

impact of a piston.[4] An experimental study was subsequently carried out, in which the propagation of high-amplitude compressional waves in a chain of beads in Hertzian contact was investigated.[5] An extensive range of pulse amplitudes was used, with the chain submitted or not to a small pre-compressional static force. Comparison of the shape and velocity the solitary waves as functions of their maximum amplitude yielded good agreement with results from the discrete mechanics model.

The study of nonlinear phenomena in granular chains has recently been extended to biomedical applications.[9,10,11] Spadoni and Daraio[9] generated high-amplitude focused acoustic pulses using a one-dimensional array of granular chains. An investigation was conducted where the amplitude, size, and location of the focus could be controlled by varying the static pre-compression of the chains. Yang *et al.* employed granular chains to assess the structural integrity of orthopedic implants.[10] In the study described by Hutchins *et al.*[11], displacements of the order of 1 µm were produced by a resonant 73 kHz ultrasonic source to drive a granular chain consisting of six 1 mm diameter chrome steel spheres. The final sphere of the chain was in contact with a fixed support. Travelling solitary wave impulses were observed, which were due to both nonlinearity between adjacent spheres and reflections within the chain. The axial velocity of the final sphere of the chain was measured using a laser vibrometer. The acquired waveforms showed a train of impulses possessing both high amplitude and wide bandwidth, and featuring spectral content up to 200 kHz. This work was subsequently expanded upon to study the response of granular chains to a narrow band ultrasonic source, as a function of the static pre-compression of the chain, and of its properties.[12] A transduction mechanism based on the nonlinear dynamics of granular chains may in fact possess distinct features that could make it attractive to

both therapeutic high-intensity focused ultrasound applications and diagnostic applications. [11,12]

Discrete mechanics models such as the one proposed by Lydon et al.[13], have been shown to replicate features of the experimentally observed dynamics of granular chains.[5,6,11,12] Nevertheless, such models are likely to have limitations when it comes to designing, developing and optimizing application-specific transducers. Indeed, in the case of biomedical ultrasound applications, a granular chain may include other components, such as a 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 behavior. An investigation into generating acoustic signals suitable for biomedical applications will involve the study of how the acoustic medium will couple to the granular chain and how resulting acoustic signals will propagate. These complexities suggest that a numerical solution to the design of such a transducer is likely to provide more flexibility than the widely used discrete mechanics models.

Khatri et al.[15] developed a finite element model using the Abaqus software to simulate the dynamic behaviour of nonlinear actuator system based on tunable granular chains, consisting of rods terminated by a linear elastic rod. Good agreement with the discrete mechanics solution and with experimental results was demonstrated. Musson and Carlson[16] carried out a finite element analysis (FEA) of the nonlinear dynamics of the granular chain investigated in by Lazaridi and Nesterenko.[4] This solution was provided by the COMSOL Multiphysics software. It was shown that FEA could successfully model the generation of solitary waves in a chain of 20 beads.

Furthermore, the FEA results demonstrated the importance of localized plastic deformations in the dynamics of granular chains, hence addressing a limitation of discrete mechanics models, where plastic deformations are neglected, as the beads are assumed to be point masses.[5] A finite element model was also developed to simulate the propagation of a solitary wave in a granular chain, in contact with a cement sample.[17] Based on the characteristics of the observed reflected wave, an assessment of the elastic properties of the cement is reported. The above studies generally focus on the simulation of solitary wave propagation as a result of a single impact onto the first bead of the granular chain. Based on the results reported by Hutchins et al.[11,12] there is a requirement to extend FEA to higher frequency excitation signals, in order to develop a better understanding of how the nonlinear characteristics of granular chains may be harnessed to develop novel biomedical devices. Whilst the physics governing the systems under investigation remain the same, the computational challenges are more substantial owing to the high frequency content of the signals relative to the dimensions of the granular chain. Resolving this frequency content is likely to involve increasingly finer meshes and smaller time-steps. In order to address these issues, a preliminary study was described by Gélat et al.[18], where FEA was used to study the behavior of a six-bead granular chain subject to sinusoidal excitation. The granular chain described by Hutchins et al.[11] was subjected to five cycles of a sinusoidal displacement of 0.3 μm amplitude, via a rigidly vibrating cylindrical piston at a frequency of 73 kHz. Displacements at the center of each bead were obtained as a function of time and compared with results from the discrete mechanics model described by Lydon et al.[13], as implemented by Hutchins et al.[11], and in absence of any viscous damping. The FEA results were in good overall agreement with the discrete mechanics model and successfully resolved multiple collisions between the

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beads. Discernible differences between the FEA and the discrete mechanics solution 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 this paper, the preliminary model described by Gélat et al.[17] was further developed to include an annulus-shaped support made of liquid photopolymer resin, which was contact with the last bead of the granular chain. This is representative of what has been used experimentally by Hutchins et al.[11] Dissipation mechanisms due to viscoelastic losses were implemented through the use of viscous dampers connected between the beads. The first sphere of the chain was excited via a rigidly vibrating cylindrical piston, the axial displacement of which was obtained from a laser vibrometer measurement at the tip of the purpose-built piezoelectric horn ultrasonic transducer described by Hutchins et al.[11] The fundamental frequency of the voltage excitation signal was 73 kHz and this resulted in a peak normal tip displacement magnitude of 1 μm. The FEA was carried out using a transient analysis in ANSYS Mechanical version 16.1.[18] The chain was subsequently coupled to a half-space of water via a thin layer of vitreous carbon and the acoustic pressure 1 mm from the fluid/structure interface resulting from the harmonic excitation of the granular chain, was computed.

II.   METHOD

A. Discrete mechanics formulations

Linear elasticity provides an exact solution to the static frictionless interaction between two adjacent elastic spheres. This is known as Hertz's law[20], which effectively expresses a nonlinear relationship between the force F_0 exerted on the

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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

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

E and v are respectively Young's modulus and Poisson's ratio corresponding to sphere material. It should be noted that this nonlinear relationship results purely from geometrical effects and is not a result of nonlinear stress-strain relations.

Consider the case of dynamic excitation of a chain of N identical, perfectly aligned spheres in Hertzian contact. If it is assumed that the 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, equation (1) can be considered valid for dynamic excitation.[6] The dynamics of the ith bead of the granular chain can then be expressed as follows:[6]

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

Equation (3) can account for loss of contacts between the beads by noting that only positive arguments of the 3⁄2 power-law terms need be considered. When the beads lose contact, i.e. for tensionless behavior, these terms can be set to zero for negative values of these arguments. Initial validation of the FEA was carried out in using the

above discrete mechanics formulation,[18] as implemented by Hutchins *et al.*[11] Validation of the FEA with equation (3) will also be presented in this paper. It is felt that such further validation is desirable as granular chains are inherently highly nonlinear systems, and the displacement excitation acting on the first sphere of the chain is in this case over three times higher in magnitude than used by Gélat *et al.*[18]

B. Finite element analysis

The problem of frictionless (Hertzian) contact between two solid bodies is commonly expressed as a variational inequality. This poses a special type of minimization problem with inequality constraints, which can be efficiently treated with (a) the penalty method, (b) the augmented Lagrangian method or (c) the Lagrange multiplier method.[21] An in-depth explanation of these methods is presented by Yastrebov.[21] In this paper, the Lagrange multiplier method as implemented in ANSYS[TM] Mechanical v16.1 FEA package was used to solve the minimization problem associated with contacts between adjacent spheres and with the piston and support. Reasons for this are discussed by Gélat *et al.*[18]

In simulations where the granular chain was coupled to an acoustic medium, the propagation of acoustic waves inside the fluid was assumed to be governed by the linear, inviscid acoustic wave equation, so that the fluid could be defined in terms of its equilibrium density and speed of sound. Coupling at the fluid/structure interface assumed continuity of normal velocity. An absorbing boundary was placed around the acoustic finite element mesh in order to simulate the Sommerfeld radiating condition and propagation of acoustic waves into a half-space.

C. Experimental configuration

The experimental displacement normal to the horn transducer tip was measured using a laser vibrometer. The measurement protocol, which is further described by Hutchins et al.[12] and by Omololu et al.[13], is summarized below.
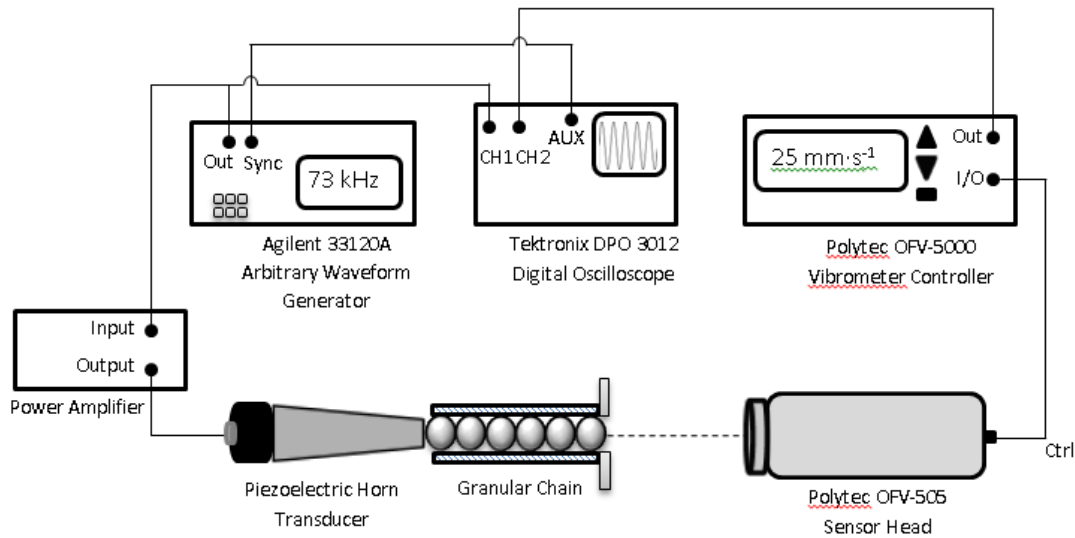

Fig. 1. Schematic diagram of the experimental configuration used for the acquisition of granular chain displacement signals.

The experimental arrangement used is shown in Fig. 1. Six spheres of 1 mm diameter chrome-steel spheres were placed within a cylindrical holder made of acrylic resin and manufactured using micro-stereolithography. The spheres were placed horizontally within the holder so as to just touch each other, thus minimizing static pre-compression forces. The first sphere was excited harmonically by a longitudinal ultrasonic horn, operating at 73 kHz, which was driven by a high voltage tone-burst signal using an Agilent 33120A function/Arbitrary waveform generator and a power amplifier. Both the horn and the chains of spheres were clamped rigidly onto an optical translation stage. A micrometer was used to position the horn against the first sphere of the granular chain with as little force as possible. The last sphere of the chain was held in place using an annular aperture, allowing detection of the particle

velocity waveform at the output via a Polytec laser vibrometry system. The tone-burst duration and amplitude of the drive voltage signal could both be adjusted. The axial displacement of the horn transducer tip as a function of time is displayed in Fig. 2a. The normalized FTT of the displacement time history is displayed in Fig. 2b, demonstrating that the spectral content is essentially concentrated around the fundamental frequency of 73 kHz. It should be noted that this measurement was carried out in absence of any mechanical loading on the transducer tip. In practice, the mechanical loading induced by coupling with the granular chain is likely to result in a modified displacement time history acting on the first bead of the chain, which could constitute a source of uncertainty when comparing the modeling results with experimental data.
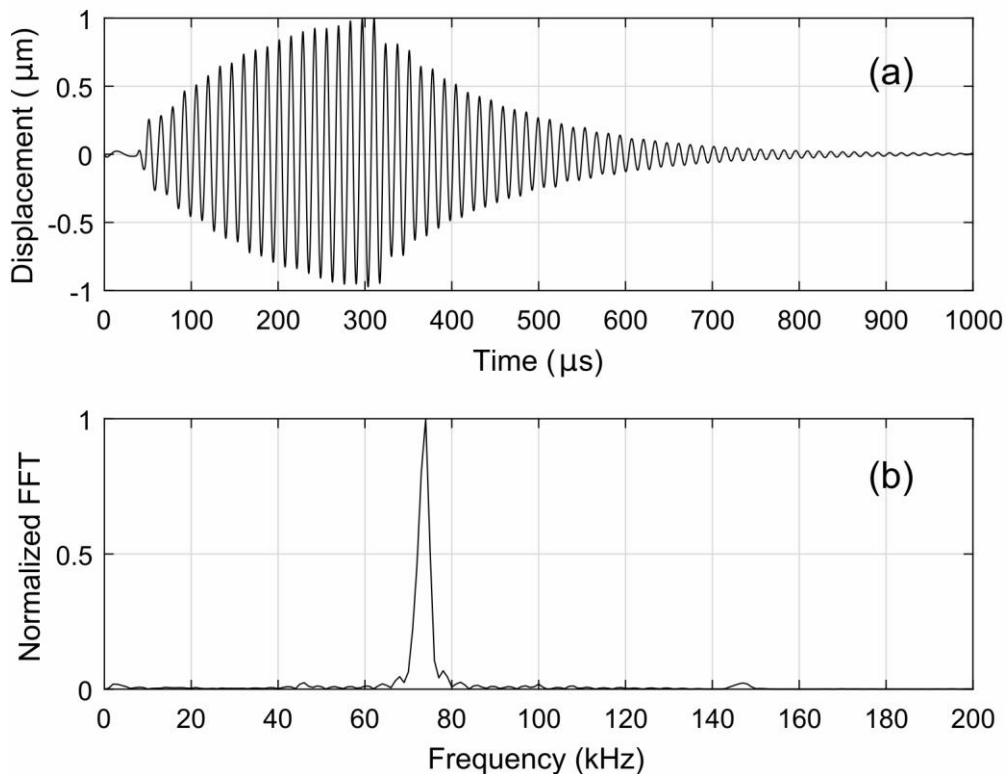

Fig. 2. (a) Normal displacement measured at the tip of the 73 kHz horn transducer using a laser vibrometer. (b) Corresponding Normalized FFT.

III. NUMERICAL CALCULATIONS

It was assumed that the beads of the granular chain were perfectly aligned. By virtue of this assumption, the configuration may be considered axisymmetric. The Cartesian y-axis was assumed to be the axis of symmetry of the chain. In the purely structural FEA calculations reported in this paper, a combination of eight node quadrilateral and six node triangular axisymmetric elements were used, with quadratic shape functions. These elements feature two translational degrees of freedom per node. All degrees of freedom of the cylindrical piston exciting the first sphere of the chain were coupled, so that they assumed the same motion along the axis of the chain, i.e. the Cartesian y-axis. In the simulations involving fluid/structure coupling, linear elements were used in the acoustic medium, as ANSYS does not allow for quadratic acoustic elements. The acoustic elements possess one degree of freedom, i.e. acoustic pressure. A 0.25 mm thick cylindrical layer of vitreous carbon of 2 mm diameter was used to couple the chain to the region of fluid, which was meshed using linear four node quadrilateral elements. The piston translational degrees of freedom along the Cartesian x-axis were restrained. A graded meshing strategy was employed, with substantial mesh refinements occurring near the contact surfaces, to ensure a smooth distribution of contact stresses.[16,17,18] A coarser mesh was allowed for at other locations to ensure that the total amount degrees of freedom could be kept within a reasonable limit, so that run times on the computing platform used would be manageable. The time step in the transient analysis was set to 0.1 μs.

In the experiments carried out by Hutchins *et al.*[11] the authors report that efforts were made to minimize pre-compressive forces. As such, the granular chain was not pre-compressed by a static force in the work described this paper. The response of the

chain to dynamic excitation as a function of a static pre-compressive force acting along the axis of the chain has been reported by Hutchins *et al.*[12]

A. FEA of granular chain terminated by a rigid support

A chain of six perfectly aligned chrome steel spheres was excited with five cycles of a 73 kHz, 1 μm amplitude sinusoidal displacement waveform. The final sphere of the granular chain was in contact with a rigid support. All contacts were assumed to be frictionless. This analysis was carried out primarily as a validation exercise, to investigate the agreement of the FEA with the discrete mechanics model implemented by Hutchins *et al.*[11]

The mesh used for analysis of the dynamics of the six-bead granular chain involving a rigid support is shown in Fig. 3. The properties of chrome steel were defined by a Young's modulus of 201 GPa, a density of 7833 kg·m^{-3} and a Poisson's ratio of 0.3.[11]
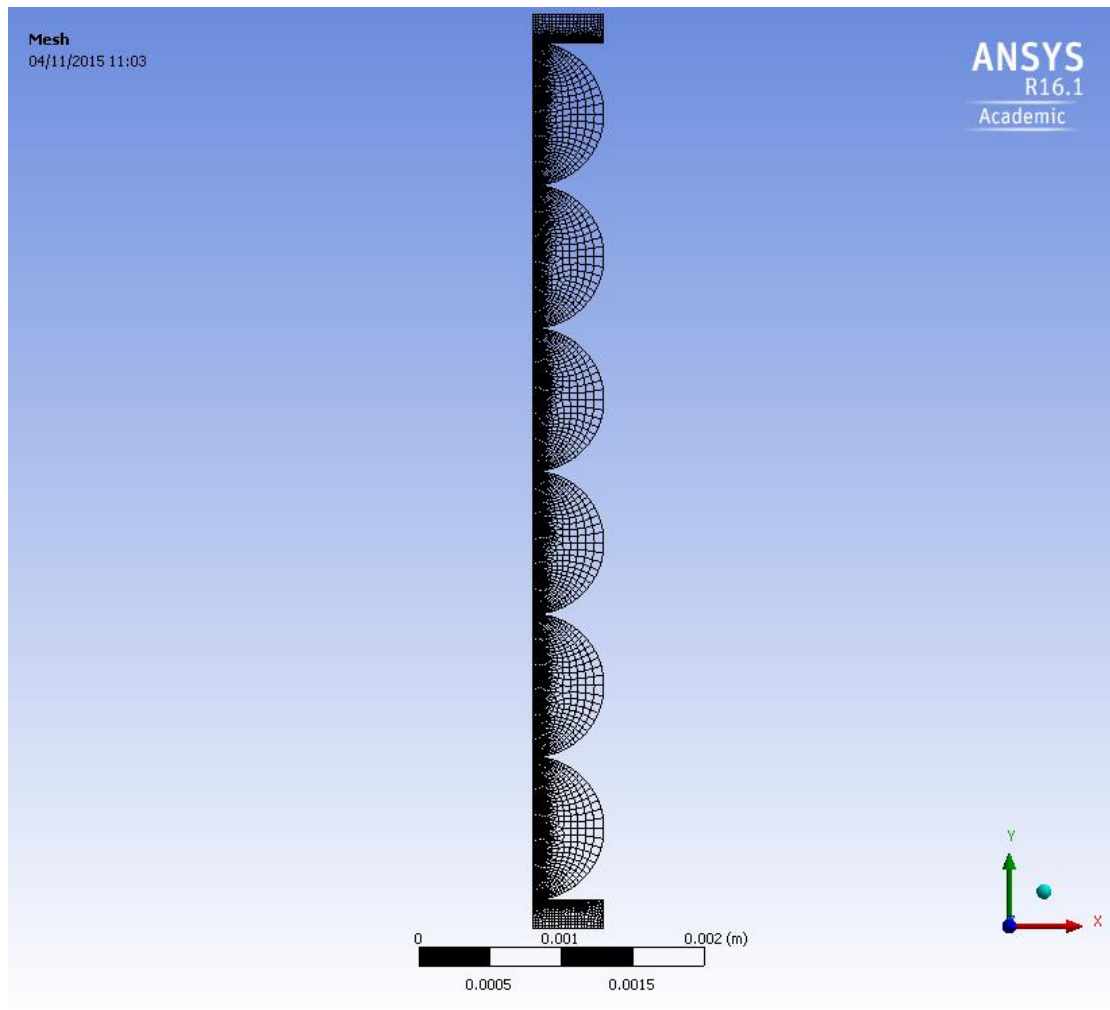
Fig. 3. Mesh used for axisymmetric FEA of six-bead granular chain. The top-most sphere is excited by a rigidly-vibrating cylindrical piston. The bottom-most sphere is in contact with a rigid support. 3038 contact elements; and 7477 solid elements were used.

B. FEA of a granular chain terminated by an annular support

A transient dynamic analysis was carried out using the displacement time history obtained from laser vibrometry, which was used as input data for the Cartesian y-component of the displacement of the piston cylinder. The geometry of the annular support in contact with the final sphere of the chain was based on that used experimentally by Hutchins et al.[11] The annulus has an outer diameter of 0.55 mm and an inner diameter of 0.3 mm. Its thickness along the Cartesian y-direction is 0.5 mm. The outer surface of the annular support was assumed to be rigidly clamped. The

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surface of the support in contact with the final sphere of the chain was modified to avoid defining a contact region involving a sharp edge, as this is known to cause numerical instability[19]. A toroidal surface was assumed, which results in a semi-circle of radius 0.25 mm in the *x-y* plane. The mesh used for the FEA of the six-bead granular chain involving an annular support is shown in Fig. 4.
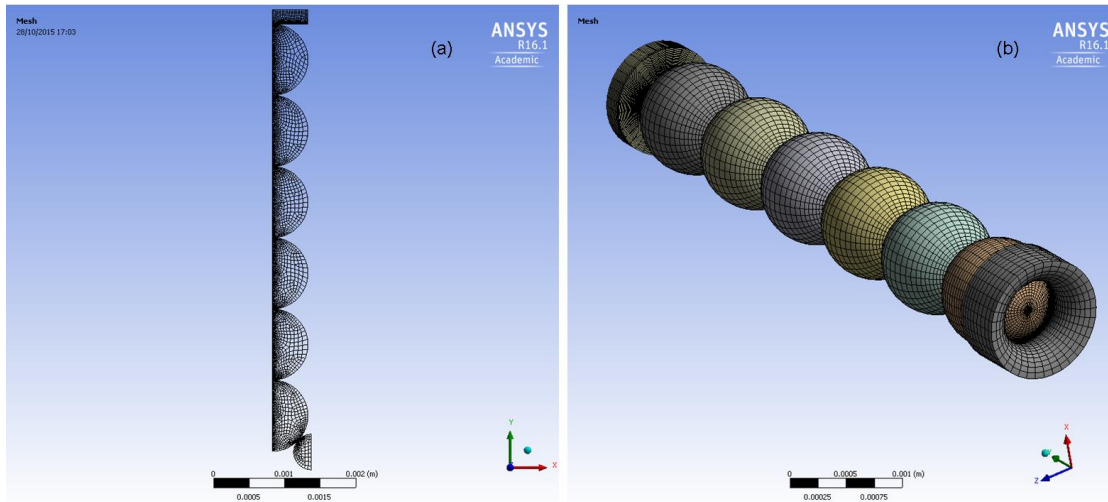

Fig. 4. (a) Mesh used for axisymmetric FEA of six-bead granular chain. The top-most sphere is excited by a rigidly-vibrating cylindrical piston. The bottom-most sphere is in contact with an annular liquid photopolymer resin support, clamped at its outer diameter. 2267 contact elements; and 5397 solid elements were used. (b) Three-dimensional visualization of mesh used for axisymmetric FEA of six-bead granular chain, cylindrical piston and annular support.

The support was assigned the properties of EnvisionTEC[TM] R11 liquid photopolymer resin, which were obtained from the manufacturer's datasheet[22]. A value of Young's modulus of 1.4 GPa was used. The density of the support was taken as 1235 kg·m^{-3} and Poisson's ratio 0.35. Dissipative effects in the granular chain include, but are not limited to, viscoelastic losses as adjacent bodies collide and frictional contact of the spheres with the holder wall. To address the latter, a full three dimensional model would be required, as the holder inner diameter is slightly larger than that of the spheres (to allow for movement of the beads). Hence, in practice, the spheres are not

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perfectly aligned. Such a model would introduce additional complexities and is beyond the scope of the work described in this paper. In the calculations in this paper, the dissipative mechanisms were limited to viscoelastic damping. Two types of viscoelastic damping models were considered. One based on a velocity proportional damper and the other based on a nonlinear formulation proposed by Kuwabara and Kono.[22] The latter effectively involves a damping coefficient proportional to the square root of the distance of approach between two adjacent spheres of the chain as they collide. It was chosen to implement this formulation as it features good representation of coefficients of restitution for hard metallic materials.[24] A value of 0.3 N·s·m^{-1} was used for the damping coefficient of the dashpots in the velocity proportional dashpot model. Comparisons with the experimental results by Hutchins *et al.*[11] were used as a guideline to choosing this value, where the peak positive value of the measured normal velocity of the last sphere of the chain was used a reference. The authors acknowledge that this approach is heuristic in nature. In the nonlinear formulation proposed by Kuwabara and Kono[23], a value of $3.66 \cdot 10^3$ N·m$^{-3/2}$ was used for the dissipative factor of chrome steel, as derived from a least squares fit by Kruggel-Emden *et al.*[23] In both implementations, as adjacent spheres separated, the damping term was set to zero. This was implemented by monitoring the positions of the centers of the spheres at each time step of the analysis.

IV. RESULTS

A. Granular chain terminated by a rigid support: FEA results

Fig. 5 displays the *y*-component of the velocity at the center of the final sphere of the granular chain as a function of time, with the chain terminated by a rigid support. As described in Section III, the piston axial displacement time history consisted of five

cycles of a 73 kHz sinusoidal waveform. Results for both the FEA and the discrete mechanics model are shown in Fig. 5, in which good agreement between both models is shown. This provides confidence in the protocol used in the FEA modeling, in terms of the mesh density, the chosen time step and the overall accuracy of the solver.
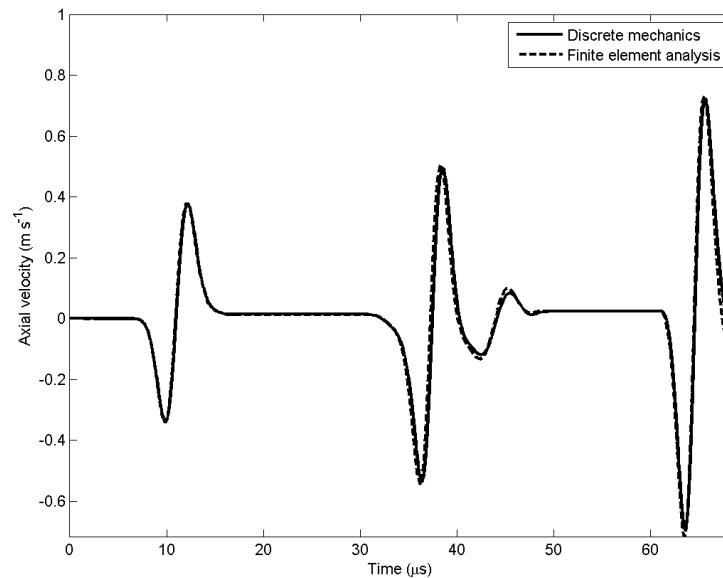

Fig. 5. Axial component of the velocity at the center of the final sphere of the granular chain terminated with a rigid support. Comparison of FEA and discrete mechanics solution.

B. Granular chain terminated by an annular support: structural FEA results and validation

Fig. 6a shows the time domain velocity of the last bead of the granular chain measured using a laser vibrometer, when the first sphere was excited using the horn transducer used by Hutchins *et al.*[11,12] Fig. 6b displays the normalized FFT of the velocity signal. Both these results have already been published[11] and are reproduced here for comparison purposes.
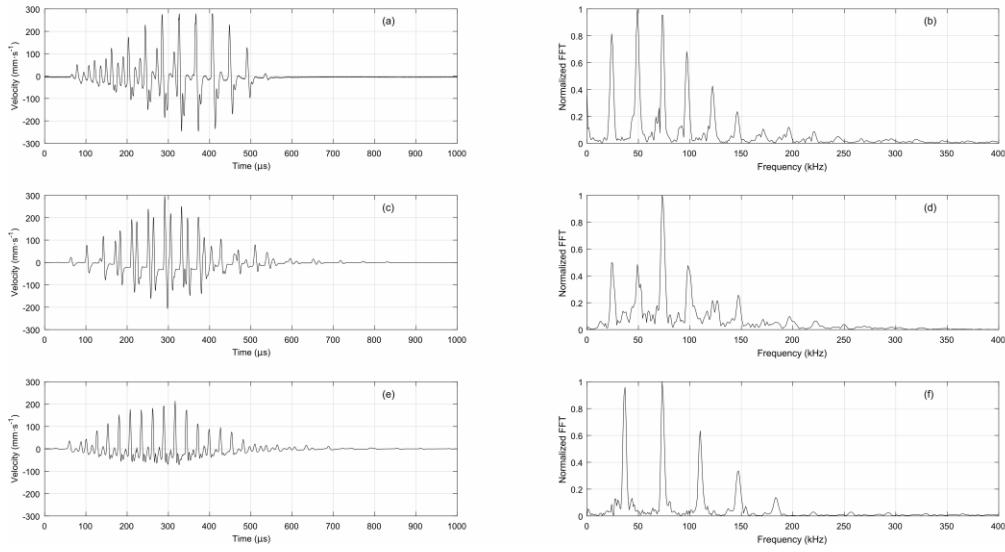
Fig. 6. Axial component of the velocity at the pole of the final sphere of the granular chain (a) measured using a laser vibrometer, (c) predicted with FEA using velocity proportional damping coefficients and with an excitation displacement corresponding to the waveform in (a) scaled by 0.5, and (e) predicted with FEA using a nonlinear damping coefficients based on the formulation by Kuwabara and Kono[22] and with an excitation displacement corresponding to the waveform in (a) scaled by 1.5. (b), (d) and (f) correspond to the normalized FFTs of the waveforms in (a), (c) and (e), respectively.

It has been demonstrated by Hutchins *et al.*[12] that these types of impulses generated by exciting a six-bead granular chain were only created when the experimental conditions were correctly fine-tuned, an important parameter being the input waveform amplitude. It was noted in Section II C that there exists uncertainty in the normal displacement acting on the first sphere of the chain, since this quantity was measured without any mechanical loading of the chain on the transducer. Furthermore, due to the fact that the system under investigation is stongly nonlinear, its output is likely to be highly sensitive to initial conditions. In order to reflect this uncertainty, a sensitivity analysis to the input displacement was carried out. The amplitude of the input displacement which described the cylindrical piston motion

was multiplied by a scaling factor α which was varied between 0.3 and 1.5, in steps of 0.05. For each value of α, the velocity of the final sphere of the chain obtained using FEA. It was observed that for $\alpha = 0.5$, the ratio of magnitude of the harmonic at 24.3 kHz to that of the fundamental frequency for this velocity reaches a maximum when the dissipative effects were assumed to be represented by velocity proportional dampers. Fig. 6c shows the axial velocity time history at the pole of the final sphere of the granular chain, predicted by the FEA. This location corresponds to that at which the laser vibrometer measurement was carried out by Hutchins et al.[11] The velocity time history replicates features of the laser vibrometer measurement reported by Hutchins et al.[11] Indeed, a similar train of impulses is predicted here using FEA. Furthermore, the peak positive and peak negative amplitudes are respectively 296 mm·s^{-1} and −207 mm·s^{-1} and the corresponding experimental values are 289 mm·s^{-1} and −247 mm·s^{-1}. The FFT of the velocity waveform in Fig. 6c is displayed in Fig. 6d. Fig. 6d shows that the frequency content of the axial velocity of the final sphere of the chain bears particular features. Whilst there remains spectral content at 73 kHz, harmonics at 1/3rd and 2/3rd of this frequency are also observed, together with ultraharmonics of these spectral components. Such features were reported by Hutchins et al.[11,12] where it was shown that this behavior was dependent on the excitation magnitude, the number of beads in the chain and on how the latter was terminated.

Another similar sensitivity analysis was carried out where the dissipative effects were represented by the nonlinear dampers proposed by Kuwabara and Kono.[22] All other model parameters remained unchanged. Whilst the axial velocity of the final sphere of the chain was shown to result in a train of impulses, its time and frequency domain characteristics were distinct from those obtained when using velocity proportional

damper. The set of results that best matched the experimental behavior in terms of the peak positive velocity was for $\alpha = 1.5$. The velocity waveform of the last sphere of the chai and its normalized FFT are displayed in Figs. 6e and 6f, respectively. Although Fig. 6e shows a peak positive velocity of 214 mm·s^{-1}, the peak negative velocity is -71 mm·s^{-1} which is proportionally much lower than the experimental value in Fig. 6a. Additionally, the spectral content displayed in Fig. 6f shows that the waveform in Fig. 6e has harmonics at half rather than 1/3rd and 2/3rd of the fundamental frequency.

The signals predicted by the FEA which most closely match those observed by Hutchins et al.[11] are those in Fig. 6c, which were obtained using velocity proportional dampers. Prior studies have demonstrated that dissipative effects due to viscoelasticity in granular chains of chrome steel beads may be more closely approximated by nonlinear damper models.[24] It appear that, however, in this case, velocity proportional dampers provide better agreement with experimental results. There exist sources of dissipation other than viscoelasticity, including friction with the holder, plasticity of the beads, and viscous drag.[1] It is therefore possible that a more simplified model for damping in fact results in a better heuristic description of the overall mechanisms for dissipation. Clearly, further simulations and experimentation would be required to confirm this. The effects of von Mises stresses and their impact on plasticity have been studied using FEA by Musson and Carlson[16] demonstrating that localized plastic deformation is a likely source of dissipation in the experiments carried out by Lazaridi and Nesterenko[4]. This is also likely to be the case in the experiments described by Hutchins et al.[11,12] Friction of the beads with the cylindrical holder is also likely to be a source of dissipation, as is viscous drag. The inclusion of such effects was considered beyond the scope of the study. It is however acknowledged that all the

above phenomena, together with imperfect experimental alignment of the beads and indeed the elasticity of the holder, will play a role in the observed discrepancies between experimental and FEA results. This statement is supported by a recent study whereby, in granular chains featuring stainless steel beads of 0.3 mm diameter, it was demonstrated that the propagation of highly nonlinear solitary waves was very sensitive to the presence of imperfections, including misalignment of the beads.[25]

Whilst Figs. 6c and 6d bear similar features to Figs. 6e and 6f, respectively, some discrepancies between the FEA and experimental results exist. Indeed, the spectral content in the vicinity of 1/3rd and 2/3rd of the fundamental frequency is more pronounced in the experimental case. Due to the high nonlinearity of the system being studied, it is somewhat expected that differences between experimental observation and theoretical calculations should exist, due to propagation of uncertainties in the system as time increases. In addition to the methodology used for modelling mechanisms of dissipation, which has been discussed in the previous paragraph, two other important sources of uncertainties are present. The first is related to the pre-compression of the granular chain. In practice, some pre-compression will always be present when coupling the transducer to the first sphere of the chain. Prior theoretical[5] and experimental[12] studies demonstrate that this is an important parameter which has a strong effect on the dynamics of the chain. The second source of uncertainty, which was mentioned in Section IIC, is the effect of the mechanical loading of the granular chain on the vibration of the horn transducer tip. Hence, the input displacement waveform shown in Fig. 2a may not in fact be entirely representative of how the chain is excited, and is likely to be overestimated. The sensitivity analysis carried out here confirms this observation.

Another class of uncertainties arises from effects of particle rotation. In point bodies representing a continuum, a generalized theory of elasticity accounting for the rotational degrees of freedom of these bodies was proposed.[26] Experimental observation of coupled rotational-translational modes in 3D, hexagonal closely packed granular phononic crystals has been recently carried out.[27] Experimental evidence of transverse rotational modes has also been observed in a 1D magneto-granular phononic crystal, with beads of 15.875 mm diameter.[28] Effects of nonlinear dynamic hysteresis, such as nonlinear absorption, have been shown to occur in granular chains under torsional excitation.[29]

Whilst the experimental configuration and excitation conditions reported above differ somewhat from those described in this paper, these particle rotation and nonlinear hysteretic effects could constitute a further source of discrepancies between FEA and experiment, since the FEA is limited to the axisymmetric case. In practice, due to manufacturing tolerances, the horn transducer used in the experiments described in this paper is unlikely to result in a tip displacement which is purely translational. Thus, contributions from undesirable rotational excitations could distinctly affect the dynamics of the granular chain. Further research is however required to clarify the extent to which this occurs relative to other unwanted effects. Quantifying these effects could be particularly important when designing clinical devices where a reproducible output within strict tolerances is required.

C. Acoustic pressure prediction using FEA

Following the results in the previous section, it was decided that the velocity proportional damping model provided a better description of the experimental configuration. It was therefore used in the FEA involving fluid/structure coupling, the

outcome of which is discussed in this Section. The six-bead granular chain under investigation was coupled to a half-space of a fluid via a 0.25 mm thick cylindrical layer of vitreous carbon. A displacement excitation was applied to the steel piston in contact with the first sphere of the granular chain, with a fundamental frequency of 73 kHz. The displacement signal consisted of a 30 cycle sinusoidal waveform with a Gaussian envelope. A sensitivity analysis was carried out, similar to that described in Section IV B, where the amplitude of the driving signal was varied until the desired train of impulses was generated. Such signals were observed for a peak displacement of 3.96 μm. The input displacement signal and its normalized FFT are shown in Fig. 7.
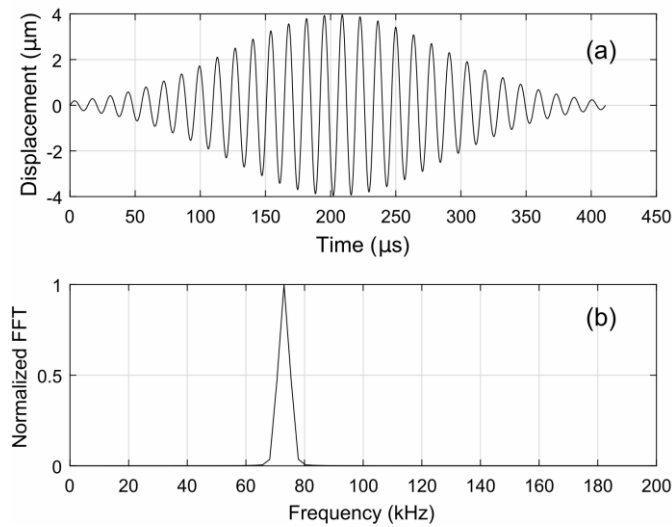

FIG. 7. (a) Piston excitation displacement waveform used for acoustic pressure predictions. 73 kHz fundamental 30-cycle sinusoidal pulse with a Gaussian envelope and with a peak value of 3.96 μm. (b) Corresponding normalized FFT.

The density of the acoustic medium was 1000 kg·m^{-3}. The speed of propagation of compressional waves was 1500 m·s^{-1}. The properties of vitreous carbon were those of Sigradur® K i.e. a Young's modulus of 35 GPa, a density of 1540 kg·m^{-3} and a

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Poisson's ratio of 0.15. The velocity of the final sphere of the chain, in contact with the vitreous carbon cylinder, was extracted from the FEA. The acoustic pressure was predicted 1 mm from the fluid/structure interface, along the axis of symmetry of the configuration. These results, along with the normalized FFT of the acoustic pressure signal, are shown in Fig. 8a, 8b and 8c, respectively.
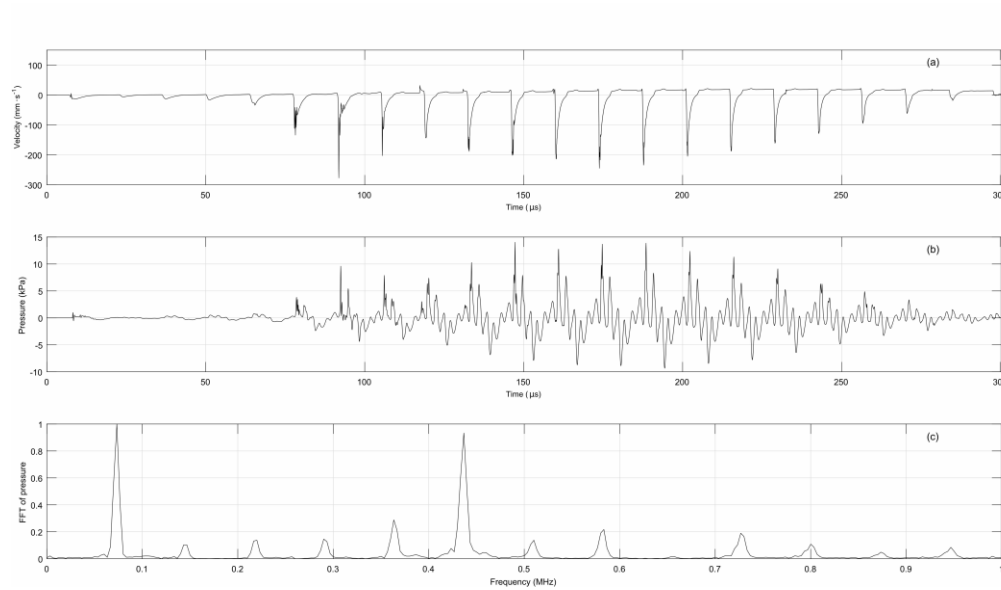

FIG. 8 (a) Axial component of the velocity at the pole of the final sphere of the granular chain, in contact with the cylindrical layer of vitreous carbon. (b) Acoustic pressure predicted with FEA 1 mm from the fluid/structure interface on the axis of symmetry. (c) Normalized FFT of acoustic pressure waveform in (b).

This set of results clearly shows that a pulse train is propagated into the acoustic medium, with a peak acoustic pressure of 14 kPa, 1 mm from the fluid/structure interface. The acoustic signal has multiple harmonics and features spectral content up to 0.95 MHz, at −21 dB relative to the fundamental frequency. This set of results demonstrates the potential for generating acoustic signals with frequency content of relevance to biomedical ultrasound applications.

V. CONCLUSIONS

In this paper, a finite element contact mechanics model was presented for simulating the dynamics of a granular chain, subjected to a tone burst excitation. The model was initially validated against results from a discrete mechanics model commonly used to simulate the dynamics of chains of spheres in Hertzian contact. A rigid support was used to terminate the chain in this validation exercise, as this could be replicated in the discrete mechanics model. Good agreement between both models was obtained. The FEA model was subsequently modified to include an accurate model of the termination of the granular chain used in the experiments carried out by Hutchins *et al.*[11] This termination consisted of an annular support made of a liquid photopolymer resin, rigidly clamped around its outer diameter. The predicted axial component of the velocity of the final sphere of the chain was compared with the laser vibrometer measurement obtained by Hutchins *et al.*[11] Two types of viscoelastic damping models were implements: one based on velocity proportional damping and another featuring a nonlinear damping coefficient proportional to the square root of the distance of approach between the centers of two adjacent spheres. The former provided good agreement with the experimental waveform both in terms of its time domain and frequency domain characteristics. The finite element model was then extended whereby the granular chain was coupled to a half-space of water via a thin layer of vitreous carbon. Under specific excitation conditions, it was possible to generate frequency content close to 1 MHz with a 73 kHz fundamental excitation signal on the first sphere of the chain.

This work was carried out in view of simulating a transduction mechanism which is of interest to biomedical ultrasound applications, whereby a narrowband excitation can

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result in high-amplitude impulses which possess a broad range of frequencies. The analyses presented in this paper demonstrate that, despite the strong nonlinearities present in the dynamics of the system under investigation, FEA is a suitable tool for predicting both time and frequency domain features of transmitted ultrasonic signals. Applications of the resulting acoustic signals may then be studied for a range of biomedical ultrasound applications. These include therapeutic ultrasound, medical imaging and targeted drug delivery. FEA will enable configurations which present challenges using discrete mechanics formulations to be investigated thoroughly, and suitable transducer designs arrived at.

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