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TAPPING DYNAMICS FOR A COLUMN OF PARTICLES AND BEYOND

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This paper is respectfully dedicated to Marie-Louise and Charles Steele.

The dynamics of a vertical stack of particles subject to gravity and a sequence of small, periodically applied taps is considered. First, the motion of the particles, assumed to be identical, is modeled as a system of ordinary differential equations, which is analyzed with an eye to observing connections with finite-dimensional Hamiltonian systems. Then, two approaches to obtaining approximate continuum models for large numbers of particles are described: the long-wave approximation that yields partial differential equations and the BSR method that employs integro-partial differential models. These approximate continuum models, which comprise infinite-dimensional dynamical systems, are studied with a focus on nonlinear wave type behavior, which naturally leads to investigating links to infinite-dimensional Hamiltonian systems. Several examples are solved numerically to show similarities among the solution properties of the finite-dimensional (lattice-dynamics), and the approximate long-wave and BSR continuum models. Extensions to higher dimensions and more general dynamically driven particle configurations are also sketched.

1. Introduction

There are several extant explanations of the dynamical behavior of configurations of particles subjected to small periodic tapping forces, most of which are aimed at conforming to a number of empirically derived formulas currently in use. Our primary intention is to apply fundamental principles of physics to obtain dynamical models for the evolution of systems of particles subjected to such tapping perturbations, and from them deduce simpler dynamical models - accessible to modern dynamical systems analysis — that are capable of predicting some of the most important aspects of the evolution of these systems with acceptable accuracy. Two of our main tools shall be the long-wave limit procedure, which has been successfully applied to particle dynamics by researchers such as Nesterenko, Daraio and their collaborators [Daraio et al. 2006; Nesterenko 1983; Nesterenko et al. 2005; Porter et al. 2009], and simplified integro-differential dynamical models developed in [Blackmore and Dave 1997; 1999; 2000]. In this regard, one should mention that there also is the related direct lattice-dynamics of FPU-chains approach of [Sen and Manciu 1999; 2001], which deals directly with the dynamics of long chains of particles, without going to a limit, and provides many opportunities for comparison with the results of the continuum approximation methods especially with regard to nonlinear wave type behavior of solutions. In addition, we shall briefly consider possible generalizations of these approximate continuum modeling

approaches to higher-dimensional tapping problems and even more general granular flow phenomena. Along the way, we shall indicate some of the most interesting dynamical systems aspects of the models that are introduced and analyze them from a more theoretical perspective.

We begin in Section 2 with a continuous one-dimensional dynamical model for the vertical column of particles (assuming Walton–Braun–Mindlin type interaction laws) expressed as a system of ordinary differential equations (ODEs) in the usual Newtonian way. The initial system of second order equations is converted to a system of first order equations emphasizing the comparison with the Hamiltonian system obtained for perfectly elastic collisions. In Section 3, we illustrate the dynamics with numerical solutions for a couple of cases with relatively small numbers of particles, and also deduce a theorem about the existence of chaotic dynamics.

Then, in Sections 4 and 5, we use this system in two different ways to obtain approximate continuum models for the tapping dynamics of a monodisperse column of particles in the form of infinite-dimensional dynamical systems comprised of partial differential equations (PDEs) or integro-partial differential equations (IPDEs). In particular, the PDEs are obtained using a standard long-wave limit, such as in [Daraio et al. 2006; Nesterenko 1983; Nesterenko et al. 2005; Porter et al. 2009; Zabusky and Kruskal 1965], as the number of particles goes to infinity, and then using the simplified model in [Blackmore et al. 1999]. A monodisperse system of particles is chosen in the interest of simplicity, since the dynamics of polydisperse systems are considerably more difficult to approximate using continuum models, especially for the long-wave limit method. After developing approximate continuum models for the tapping dynamics via the *long-wave* (L-W) and Blackmore–Samulyak–Rosato (BSR) methods, we also formulate the associated boundary-initial value problems corresponding to the one-dimensional vertical tapping regime under investigation in these sections, respectively.

In Section 6, we turn our attention to some of the mathematical properties of the L-W and BSR dynamics, with a focus on the Hamiltonian and near Hamiltonian infinite-dimensional dynamical systems associated with these continuum models. Some of the results for the approximate L-W and BSR models have already been proved in the literature, and some related theorems shall only be stated since their proofs, which shall be treated in forthcoming work, are a bit too technical to include in this paper. We follow this in Section 7 with numerical solutions of the L-W and BSR approximations corresponding to the numerical simulations of the tapping regimes considered in Section 3, and find good qualitative agreement among the solutions of the exact and both approximate continuum models. Finally, in Section 7, we summarize the work presented and outline some of our plans for future research — both with regard to granular flow applications and infinite-dimensional dynamical system theory - for higher-dimensional systems and more general particle configurations and forcing scenarios.

2. Newtonian model

We begin with a mathematical model for the tapping motion of the column of particles obtained using Newtonian and Hamiltonian principles assuming that the particle-particle and particle-floor interaction forces are of Walton–Braun–Mindlin type [Blackmore et al. 1999; MacKay 1999; Blackmore and Dave 1997; Daraio et al. 2006; Sen and Manciu 1999; Nesterenko 1983]. The results obtained have certain aspects in common with the approaches of the last four works just cited and of [Blackmore et al. 2000; Fermi et al. 1965; Nesterenko et al. 2005; Porter et al. 2009; Sen and Manciu 2001], among many

other works. In particular, we consider a configuration of N particles p_i, $1 \le i \le N$, aligned along the (vertical) positive y-axis, stacked one above the other starting with p_1, under the action of gravity — with constant gravitational acceleration g — and interacting inelastically (according to the Walton–Braun–Mindlin model) with neighboring particles and a "container" bottom, denoted as y_0, initially at the origin that is moving in a manner that simulates a periodic nearly impulsive tapping force applied vertically to the floor. The moving bottom and particle centers are located, respectively, at the points

$$0 \le y_0(t) < y_1 < \cdots < y_N \tag{1}$$

in the semi-infinite interval $I := \{y : 0 \le y\}$, and we assume that the particles have masses and radii $m_1, r_1, \ldots, m_N, r_N$, respectively.

In order to model the periodic tapping, we assume that $y_0(t)$ is a periodic function of period $T > 0$ represented as

$$y_0(t) := \begin{cases} a \sin \omega t & \text{if } 0 < t \le \pi/\omega, \\ 0 & \text{if } t = 0 \text{ or } \pi/\omega \le t \le T \end{cases} \tag{2}$$

for $0 \le t \le T$, where $\pi/\omega \ll T$, and the amplitude a is a small positive number. Note that the derivative of (2) with respect to t, denoted by a dot over the variable, is the discontinuous function given as

$$\dot{y}_0(t) := \begin{cases} a\omega \cos \omega t & \text{if } 0 < t \le \pi/\omega, \\ 0 & \text{if } t = 0 \text{ or } \pi/\omega \le t \le T. \end{cases} \tag{3}$$

Our intention is to determine the motion of the particles after each of a periodic sequence of taps, and compare the positions of the particles after being given time to settle following each of the taps — say at times $.99T$, $1.99T$, $2.99T$, ..., in order to determine trends after many such taps, with the evolution of the linear particle density being of particular interest.

We shall assume that the particles and bottom interact inelastically according to a simplified Walton–Braun–Mindlin law, so that the equations of motion obtained from Newton's second and third laws take the form of a system of N second-order ODEs:

$$m_i \ddot{y}_i = F_i \quad (1 \le i \le N), \tag{4}$$

where the forces on the particles are expressed as

$$F_i := -m_i g + f_i^{i-1} + f_i^{i+1} \tag{5}$$

for $1 \le i \le N$, where f_i^{i-1} is the force exerted by p_{i-1} (or the bottom when $i = 1$) on p_i and f_i^{i+1} is the force exerted by p_{i+1} on p_i when $1 \le i \le N - 1$. These interaction forces are given by

$$\begin{aligned} f_1^0 &:= \left(K_1^0 - \hat{K}_1^0 \sigma(\dot{y}_1 - \dot{y}_0)\right)\left(r_1 - (y_1 - y_0(t))\right)\chi\left(r_1 - (y_1 - y_0(t))\right), \\ f_i^{i+1} &:= -\left(K_i^{i+1} - \hat{K}_i^{i+1}\sigma(\Delta \dot{y}_i)\right)(r_i + r_{i+1} - \Delta y_i)\chi(r_i + r_{i+1} - \Delta y_i), \\ f_N^{N+1} &:= 0, \end{aligned} \tag{6}$$

for $1 \le i \le N - 1$, with

$$f_i^{i-1} = -f_{i-1}^i \tag{7}$$

for $2 \le i \le N$. Here

$$\Delta y_i := y_{i+1} - y_i, \quad \Delta \dot{y}_i := \dot{y}_{i+1} - \dot{y}_i, \tag{8}$$

for $1 \leq i \leq N-1$, the K_i^{i+1} and $\hat{K}_i^{i+1}$ are constants with $0 < \hat{K}_i^{i+1} \leq K_i^{i+1}$ for all $1 \leq i \leq N-1$, and σ and χ denote the signum and step functions defined, respectively, by

$$\sigma(\tau) := \begin{cases} -1 & \text{if } \tau < 0, \\ 0 & \text{if } \tau = 0, \\ 1 & \text{if } \tau > 0, \end{cases} \quad \text{and} \quad \chi(\tau) := \begin{cases} 0 & \text{if } \tau < 0, \\ \frac{1}{2} & \text{if } \tau = 0, \\ 1 & \text{if } \tau > 0. \end{cases} \tag{9}$$

With the definitions above, the system (4) may now be rewritten as

$$\ddot{y}_i = Y_i := \frac{1}{m_i} F_i = -g + \frac{1}{m_i}(f_i^{i-1} + f_i^{i+1}) \quad (1 \leq i \leq N), \tag{10}$$

which can be recast in vector form for $\boldsymbol{y} := (y_1, \ldots y_N)$ as

$$\ddot{\boldsymbol{y}} = \boldsymbol{Y}(\boldsymbol{y}, \dot{\boldsymbol{y}}, t; \boldsymbol{\mu}), \tag{11}$$

where $\boldsymbol{Y} := (Y_1, \ldots Y_N) = \left(-g + m_1^{-1}(f_1^0 + f_1^2), \ldots, -g + m_{N-1}^{-1}(f_{N-1}^{N-2} + f_{N-1}^N), -g + m_N^{-1} f_N^{N-1}\right)$, and $\boldsymbol{\mu}$ is a parameter (vector) incorporating a, ω, T, all the particle masses and radii, and all of the interaction parameters K_i^{i+1} and $\hat{K}_i^{i+1}$. As is usual for such second-order systems, we shall find it convenient to recast it as the following system of $2N$ first-order ODEs, which is better suited to direct numerical solution by such schemes as a Runge–Kutta solver:

$$\dot{y}_i = v_i, \quad \dot{v}_i = Y_i, \tag{12}$$

for $1 \leq i \leq N$. Of course, we can also write this succinctly in (the Hamiltonian related) vector form as

$$\dot{\boldsymbol{x}} = \boldsymbol{X}(\boldsymbol{x}, t; \boldsymbol{\mu}), \tag{13}$$

where

$$\boldsymbol{x} := (x_1, x_2, \ldots, x_{2N-1}, x_{2N}) := (y_1, v_1, \ldots, y_N, v_N),$$
$$\boldsymbol{X} := (X_1, X_2, \ldots, X_{2N-1}, X_N) := (v_1, Y_1, \ldots, v_N, Y_N). \tag{14}$$

Observe that only the second coordinate (component) of $\boldsymbol{X}$ depends explicitly on t, and by definition, $\boldsymbol{X}$ is periodic of period T in the independent time variable t. Also, X_2 is the only coordinate that depends explicitly on the parameters a and ω. The forces defined above are chosen so that the inelasticity of the particle-particle and particle-bottom interactions is manifested by a loss of energy upon impact that is essentially represented by a spring constant of $K_i^{i+1} + \hat{K}_i^{i+1}$ when the particles are approaching one another or the bottom and a spring constant of $K_i^{i+1} - \hat{K}_i^{i+1}$ when the particles are moving away from one another or the bottom after impact. From this perspective, the case $\hat{K}_i^{i+1} = 0$ represents a perfectly elastic interaction. We also note that the discontinuities in (13) are somewhat inconvenient from a theoretical standpoint, but they can easily be handled by a standard numerical scheme, such as a Runge–Kutta solver, and the forces can also be approximated to any degree of accuracy by smooth ($= C^\infty$) functions if necessary.

So in summary, we want to solve (13), and this can be accomplished numerically via say a variable step size Runge–Kutta scheme subject to the initial condition

$$\boldsymbol{x}(0) = (y_1(0), 0, y_2(0), \ldots, 0, y_N(0), 0), \tag{15}$$

which represents a stacked configuration of particles initially at rest. Here we have to determine the values of the $y_k(0)$ by requiring that the stack of particles is initially at rest and in equilibrium, and because the particles are assumed to be non-rigid we shall have to determine these values in a way that guarantees that $y_0(t) < y_1(t) < y_2(t) < \cdots < y_N(t)$ for all $t \geq 0$, which we shall demonstrate in the sequel for the monodisperse case. We also want to make comparisons of the positions of the particles at times, say at $.99T, 1.99T, 2.99T, \ldots, k.99T$ for rather large positive integer values of k. In these simulations it makes sense to simplify matters by taking all the $K's$ equal and all the $\hat{K}'s$ equal, with $0 \leq \hat{K} = eK$, with $0 < e < 1$, and all the radii and masses equal or having at most a pair of possible values. Note that in this context, the coefficient of restitution ϱ, which is the standard measure of elasticity with $0 \leq \varrho \leq 1$ and the left (0) and right (1) extremes representing the perfectly inelastic and elastic cases, respectively, is given as

$$\varrho^2 = \frac{1-e}{1+e}, \quad \text{or, equivalently,} \quad e = \frac{1-\varrho^2}{1+\varrho^2}. \tag{16}$$

For the other parameters, some good choices are as follows: $20 \leq N$, $T = 1$, $\pi/\omega < 1/10$, $a \leq 1/50$, $r_i = r$ and $m_i = m$, with $0 < r < 1/100$ and $0 < m < 1/20$, and it makes sense to run several cases for (13)–(15) for different parameter values satisfying these inequalities.

With the assumptions that all $K's$ and $\hat{K}'s$ are the same and $\hat{K} = eK$, the equations of motion take the form

$$\ddot{y}_i = Y_i := -g + \frac{K}{m_i}(f_i^{i-1} + f_i^{i+1}) \quad (1 \leq i \leq N), \tag{17}$$

where

$$\begin{aligned}
f_1^0 &:= [1 - e\sigma(\dot{y}_1 - \dot{y}_0(t))](r_1 - y_1 + y_0(t))\chi(r_1 - y_1 + y_0(t)), \\
f_i^{i+1} &:= -[1 - e\sigma(\Delta\dot{y}_i)](r_i + r_{i+1} - \Delta y_i)\chi(r_i + r_{i+1} - \Delta y_i), \\
f_N^{N+1} &:= 0.
\end{aligned} \tag{18}$$

Whence, the Newtonian equations of motion are

$$\begin{aligned}
\ddot{y}_1 = -g - \frac{K}{m_1}\Big(&[1 - e\sigma(\Delta\dot{y}_1)](r_1 + r_2 - \Delta y_1)\chi(r_1 + r_2 - \Delta y_1) \\
&- [1 - e\sigma(\dot{y}_1 - \dot{y}_0(t))](r_1 - y_1 + y_0(t))\chi(r_1 - y_1 + y_0(t))\Big),
\end{aligned}$$

$$\begin{aligned}
\ddot{y}_i = -g - \frac{K}{m_i}\Big(&[1 - e\sigma(\Delta\dot{y}_i)](r_i + r_{i+1} - \Delta y_i)\chi(r_i + r_{i+1} - \Delta y_i) \\
&- [1 - e\sigma(\Delta\dot{y}_{i-1})](r_{i-1} + r_i - \Delta y_{i-1})\chi(r_{i-1} + r_i - \Delta y_{i-1})\Big) \quad (2 \leq i \leq N-1),
\end{aligned} \tag{19}$$

$$\ddot{y}_N = -g + \frac{K}{m_N}[1 - e\sigma(\Delta\dot{y}_{N-1})](r_{N-1} + r_N - \Delta y_{N-1})\chi(r_{N-1} + r_N - \Delta y_{N-1}).$$

The natural initial conditions for the tapping dynamics are then

$$\begin{aligned}
&y_1(0), y_2(0), \ldots, y_N(0) \quad \text{determined by assuming initial equilibrium of column,} \\
&\dot{y}_1(0) = \dot{y}_2(0) = \dot{y}_3(0) = \cdots = \dot{y}_N(0) = 0.
\end{aligned} \tag{20}$$

It is instructive to observe that (13) can be written in the form

$$\dot{x} = \Phi(x) + \Psi(x, t; \mu), \tag{21}$$

where

$$\dot{x} = \Phi(x) \tag{22}$$

is an autonomous Hamiltonian system that is completely integrable in the Liouville–Arnold sense (*L-A integrable*) and Ψ may be viewed as a (non-Hamiltonian) perturbation of the integrable system (22) that goes to zero as $e, a \to 0$; see, for example, [Arnold 1978; Błaszak 1998; Guckenheimer and Holmes 1983; Katok and Hasselblatt 1995; Prykarpatsky et al. 1999]. We also note that the periodicity in t can be used to recast (21) in the autonomous form

$$\dot{x} = \Phi(x) + \Psi(x, \theta; \mu), \quad \dot{\theta} = 2\pi/T \tag{23}$$

on the $(2N+1)$-dimensional cylinder $\mathbb{R}^{2N} \times \mathbb{S}^1$, where $\mathbb{S}^1$ is the unit circle.

2.1. *Monodisperse particle configuration.*

In the interest of transparency and simplicity, we shall confine our attention to a monodisperse column of particles, so that we assume now and hereafter that $m_1 = \cdots = m_N := m$ and $r_1 = \cdots = r_N := r$. This assumption naturally simplifies each of the equations (17), (18) and (19); for example, (19) becomes

$$\ddot{y}_1 = -g - \frac{K}{m}\Big([1 - e\sigma(\Delta\dot{y}_1)](2r - \Delta y_1)\chi(2r - \Delta y_1) - [1 - e\sigma(\dot{y}_1 - \dot{y}_0(t))](r - y_1 + y_0(t))\chi(r - y_1 + y_0(t))\Big),$$

$$\ddot{y}_i = -g - \frac{K}{m}\Big([1 - e\sigma(\Delta\dot{y}_i)](2r - \Delta y_i)\chi(2r - \Delta y_i)[1 - e\sigma(\Delta\dot{y}_{i-1})](2r - \Delta y_{i-1})\chi(2r - \Delta y_{i-1})\Big) \tag{24}$$
$$(1 < i < N),$$

$$\ddot{y}_N = -g + \frac{K}{m}[1 - e\sigma(\Delta\dot{y}_{N-1})](2r - \Delta y_{N-1})\chi(2r - \Delta y_{N-1}),$$

and the initial conditions (20) reduce to

$$y_1(0), y_2(0), \ldots, y_N(0) \text{ to be determined} \quad \text{and} \quad \dot{y}_1(0) = \cdots \dot{y}_N(0) = 0, \tag{25}$$

and (21)–(23) are modified analogously.

To determine the initial positions, we assume that the configuration is initially at rest and in equilibrium, so (24) implies that the following equations must be satisfied:

$$-2y_1(0) + y_2(0) = r + \mathfrak{M},$$
$$y_{k-1}(0) - 2y_k(0) + y_{k+1}(0) = \mathfrak{M} \quad (1 < k < N - 1), \tag{26}$$
$$y_{N-1}(0) - y_N(0) = -2r + \mathfrak{M},$$

where

$$\mathfrak{M} := \frac{mg}{K}.$$

It is straightforward to show that (26) has the solution

$$y_k(0) = (2k - 1)r - (k/2)(2N - k + 1)\mathfrak{M} \quad (1 \le k < N - 1),$$
$$y_N(0) = (2N - 1)r - (1/2)[(N - 1)N + 2]\mathfrak{M}. \tag{27}$$

As we naturally require that $y_k(0) - y_{k-1}(0) > 0$ for all $1 \le k \le N$, this leads to the condition

$$\mathfrak{M} < \frac{r}{N}, \quad \text{or, equivalently,} \quad \frac{Ng}{r} < \frac{K}{m}, \tag{28}$$

which must be imposed in order to maintain physical realism. We note here that the maximum height S of the column of particles where they are all just touching one another is

$$S = 2Nr. \tag{29}$$

We shall study the solutions of (24)–(25) directly, and also analyze the dynamics of the corresponding first-order system (21)–(23), with the monodisperse assumption imposed to simplify the expressions. One slightly troubling feature from a theoretical standpoint is the fact is that although (20), or (24), is piecewise linear, it has jump discontinuities, which we should add can be easily handled using a numerical scheme such as the Runge–Kutta method. Theoretically, we can always adjust the systems to be smooth ($= C^\infty$) by using appropriate approximations of the signum and step functions. A rather good choice for smooth approximations is

$$\sigma(s) \cong \sigma_\alpha(s) := \tanh \alpha s, \quad \chi(s) \cong \chi_\alpha(s) := \tfrac{1}{2}(1 + \tanh \alpha s), \tag{30}$$

where $\alpha \gg 1$.

3. Dynamics of Newtonian model

In this section we shall briefly investigate the dynamical properties of the system (21) using both numerical simulation and analytical means. We begin with some numerical simulations of the solutions of (24)–(25) employing a standard ODE solver of the type used in the molecular dynamics simulation codes developed by Rosato and his collaborators, which have been applied to advantage in many studies of granular flows, such as in simulations of examples in [Blackmore et al. 1999].

For these simulations, with monodisperse particle stacks, we fix $T = 50$, $m = 1$, $r = 1.0$ cm, $a/2r = 0.53$, $e = 0.09$, $g = 980.67$ cm/sec^2, and following (29), $K = (2Ng/r)$, and vary the number of particles N over the values $N = 5, 10$. Note that the frequency $\omega = 2\pi\Gamma$ is varied for the two cases, with $\Gamma = 2.4019$ for $N = 5$ and $\Gamma = 3.8476$ for $N = 10$, mainly to obtain better resolution for the particle configurations. The dynamics for the five-particle and the ten-particle cases are illustrated in Figure 1, which plots of $y_1(t)$ through $y_N(t)$ for all choices N over a time interval long enough to include four periodic taps.
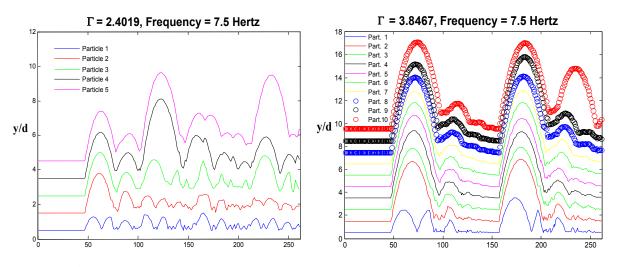

Figure 1. Particle trajectories for tapping of five (left) and ten (right) particle stacks.

Observe that in order to more clearly establish the quiescent state, the formulas for the initial conditions above are translated by 50 time steps in the numerical simulations. One can see from these time series plots for the positions of the particles how the density of the particles varies with time by observing the evolution of the interparticle distances.

From the perspective of modern dynamical systems theory, one can use the same arguments as enlisted in [Blackmore and Dave 1997; Blackmore et al. 2000] to prove the following result (see also [Guckenheimer and Holmes 1983; Prykarpatsky et al. 1999]).

Theorem 1. *Fixing all parameters save the amplitude of the taps, there exist sufficiently large values of a for which* (21) *has periodic solutions of arbitrarily large period, and ultimately there exist large values of a such that the system of particles exhibits chaotic motion. Moreover, if all the parameters are fixed but the period T of the taps, then there exist chaotic orbits when the period is sufficiently small.*

Before moving on to continuum approximations for the system (24) for very large N, we should mention a very important related body of work in the realm of lattice dynamics, which deals with a direct analysis of these equations of motion — usually focusing on finding solutions of a particular wave related form. Important representatives of this type of one-dimensional lattice dynamics research (which has yielded the existence of solitary wave solutions, solitons and breathers, to name a few examples) can be found in [Friesecke and Wattis 1994; MacKay 1999; MacKay and Aubry 1994; Poggi and Ruffo 1997; Sen and Manciu 1999; 2001; Treschev 2004; Yoshimura and Doi 2007; Zolotaryuk et al. 2000]. There are also some useful studies of the finite systems, such as in [Blackmore and Dave 1997; Blackmore et al. 2000; Yang and Wylie 2010] devoted to finding special properties of certain orbits of the dynamical systems of N particles, where N need not be particularly large.

4. Long-wave continuum approximation

We shall first use the standard long-wave continuum limit method to find an approximation for our discrete system of particles in the form of a nonlinear partial differential equation (PDE). One of the most famous examples of this approach is the continuum approximation of the Fermi–Pasta–Ulam (FPU) model [Fermi et al. 1965] obtained by Zabusky & Kruskal [Zabusky and Kruskal 1965] that established a connection between the FPU system and the Korteweg–de Vries equation that was a vital link in the chain leading to an explanation of the existence of solitons and their connection with integrable PDEs.

Toward this end, we focus on the middle equation of (24) in the monodisperse case; namely

$$\ddot{y}_i = -g - \frac{K}{m}\big([1 - e\sigma(\Delta\dot{y}_i)](2r - \Delta y_i)\chi(2r - \Delta y_i) - [1 - e\sigma(\Delta\dot{y}_{i-1})](2r - \Delta y_{i-1})\chi(2r - \Delta y_i)\big). \quad (31)$$

Next we introduce the alternative variable z for y to avoid confusion in our notation, and define $h := 2r$ to be the (mean) distance between the particles ("springs"). The underlying assumption in the long-wave approximation method is that the wavelength L of the wave phenomena embodied in the motion of the particles satisfies $h \ll L$, which as it turns out is quite a reasonable supposition for a wide range of granular flow regimes, including the one under consideration here. Our intention is to find an approximate PDE representing the dynamics of (31) as $N \to \infty$. For this we assume that y_i represents the function $y(z, t)$, which is at least of class C^4 in all of its variables, and

$$y_{i\pm 1} := y(z \pm h, t), \quad (32)$$

which can be expanded in Taylor series up to the fourth order in h as

$$y_{i\pm 1} := y(z \pm h, t) = y_i \pm y_z h + \tfrac{1}{2} y_{zz} h^2 \pm \tfrac{1}{6} y_{zzz} h^3 + \tfrac{1}{24} y_{zzzz} h^4 + \cdots, \tag{33}$$

and we also have

$$\dot{y}_{i\pm 1} := y_t(z \pm h, t) = \dot{y}_i \pm y_{tz} h + \tfrac{1}{2} y_{tzz} h^2 \pm \tfrac{1}{6} y_{tzzz} h^3 + \tfrac{1}{24} y_{tzzzz} h^4 + \cdots. \tag{34}$$

Substituting (32), (33) and (34) in (31), we find after a long and tedious but straightforward calculation that up to the fourth order in h we have the fourth order PDE on $(z, t) \in \mathbb{R}^+ \times \mathbb{R}^+ = [0, \infty) \times [0, \infty)$:

$$
\begin{aligned}
y_{tt} = -g + \frac{Kh^2}{m} \Big(& \tfrac{1}{3} A_{(+)} y_{zz} - \tfrac{1}{3} h [By_z + e\sigma'(0) A_{(+)} y_{tz}] y_{zz} \\
& + h^2 \big(\tfrac{1}{36} A_{(-)} y_{zzzz} + 2r\sigma'(0) y_z^2 y_{zz} + e\sigma'(0) By_z y_{zz} y_{tz} + \tfrac{1}{6} e\sigma'(0) A_{(+)} y_{zz} y_{tzz} \big) \Big),
\end{aligned} \tag{35}
$$

where

$$A_{(\pm)} := 3\chi(0) + 6r\sigma'(0) \pm 8r^3 \sigma'''(0) \quad \text{and} \quad B := \sigma'(0) + 4r^2 \sigma'''(0), \tag{36}$$

and we have assumed that σ and χ are convenient smooth approximations of the signum and step functions such as given in (30) and such that all even derivatives of σ and χ vanish at the origin. If we use the approximation for σ in (31), then (35) takes the form

$$
\begin{aligned}
y_{tt} = -g - \frac{Kh^2}{m} \Big(& \tfrac{1}{3} A_{(+)} y_{zz} - \tfrac{1}{3} h [By_z + e\alpha A_{(+)} y_{tz}] y_{zz} \\
& + h^2 \big(\tfrac{1}{36} A_{(-)} y_{zzzz} + \alpha (2r y_z^2 y_{zz} + e By_z y_{zz} y_{tz} + \tfrac{1}{6} e A_{(+)} y_{zz} y_{tzz}) \big) \Big),
\end{aligned} \tag{37}
$$

with

$$A_{(\pm)} := 3\chi(0) + 6r\alpha \mp 16r^3 \alpha^3 \quad \text{and} \quad B := \alpha(1 - 8r^2 \alpha^2). \tag{38}$$

We can take (37) as our long-wave continuum approximation for the dynamics of the particle system as $N \to \infty$. Note that if we choose $\chi(0) = \tfrac{1}{2}$ and $\alpha = 1/h = 1/(2r)$, then

$$A_{(+)} = 2.5, \quad A_{(-)} = 13.5 \quad \text{and} \quad B = -(1/h).$$

Observe that this is a highly nonlinear wave type equation. Of course, we shall need to impose appropriate auxiliary conditions on (35) or (37) in order to obtain well-posedness, and also include the periodic external (tapping) motion given by (2) and (3). Suitable initial and boundary conditions are

$$y(z, 0) = z, \quad y(0, t) = y_0(t), \tag{39}$$

but more has to be done in order to (approximately) model the actual evolution of the system primarily due to the vertical nature of the particle stack and the influence of gravity; something that makes analysis of a horizontal particle configuration considerably easier to handle.

We shall now briefly explain these attendant difficulties, and describe the simplified method used in this paper to deal with the intricacies of numerically solving (37). This problem is defined on the semi-infinite first quadrant of the t, z-plane in a way that actually makes it analogous to a free boundary problem that also necessitates an adjustment of the right-hand side of (37) consistent with evolution of the lower and upper boundaries of the initial "particle interval", $0 \leq y(z, 0) = z \leq S$. What is required is to find the evolution of the top point S of the vertical continuum of particle matter, $0 \leq z \leq S$, defining a

curve $z = \varphi(t)$ in the in the t, z-plane, above which the force on the right-hand side of (37) has to be set to zero. In addition, the gravity term g on the right-hand side of (37) must be set equal to zero along the moving bottom $y_0(t)$, which defines the motion of the lower boundary point of the initial particle interval. We choose to deal with these mathematical difficulties completely in a forthcoming paper dedicated to just these matters, and use a much simpler hybrid method for our numerical treatment of the solution of (37) in the sequel. In particular, we use our numerical solutions of the finite-dimensional initial value problem (24)–(25) to track the (upper) "free boundary" of the evolution of the initial particle continuum of height S, and then make the adjustments in (37) that we have just indicated.

As noted earlier, we also need to impose constraints on the parameters so that the initial stack of particles, now approximated by a continuum of height S does not collapse. To this end, noting that we are assuming $h = 2r$ to be the average distance between the particles, it follows from (27) and (28) that we must have

$$\frac{Kh^2}{m} = \frac{4Kr^2}{m} > 4Ngr = 2Sg. \tag{40}$$

So, for example, $Kh^2/m = 2.5\,Sg$ would be a safe choice.

With regard to the PDEs (35) and (37), note that they represent (infinite-dimensional) integrable Hamiltonian dynamical systems when $e = 0$ (see [Ablowitz and Segur 1981; Błaszak 1998; Blackmore et al. ≥ 2011; Dickey 1991; Faddeev and Takhtajan 1987; Prykarpatsky and Mykytiuk 1998]), which is not all that surprising since they are obtained as continuum approximations of the finite-dimensional system (21), which can be rewritten as an L-A integrable Hamiltonian system when $e = 0$.

It is useful to observe that if (37) is solved imposing the auxiliary conditions described above, we can then use the continuity equation to determine the particle density ρ via the equation

$$\frac{\partial \rho}{\partial t} + y_t \frac{\partial \rho}{\partial z} + y_{tz}\rho = 0, \tag{41}$$

subject to the auxiliary (Cauchy) condition

$$\rho(z, 0) = \text{constant} = \frac{m}{2r}. \tag{42}$$

5. Alternative continuum approximation: BSR model

There is another, more direct, method for finding continuum approximations of granular flow equations that was developed in [Blackmore et al. 1999] and used in [Blackmore and Dave 1997] to approximate the dynamics of a large number of particles moving along a horizontal line with one fixed boundary (wall) and subject to a periodic forcing function. This approach leads first to the following integro-PDE (IPDE) for the dynamics of the granular motion being considered:

$u_t + uu_z =$

$$-g - \frac{K}{m} \int_0^\infty \big([1 - e\sigma(\Delta \dot{y}_i)](2r - \Delta y_i)\chi(2r - \Delta k y_i) - [1 - e\sigma(\Delta \dot{y}_{i-1})](2r - \Delta y_{i-1})\chi(2r - \Delta y_{i-1})\big)\,dz, \tag{43}$$

where u is the velocity $y_t = z_t$. In order to obtain the correct expression for the integral, we need to reinterpret the local force (appearing as the integrand) on a particle at the point y in the manner of [Blackmore et al. 1999].

The actual force expression at $z \in [0, \infty)$, which must be "averaged" over a neighborhood $(z - y, z + y)$ corresponding to the near-neighbors in the lattice dynamics formulation in Section 2.1 is

$$-\frac{K}{m}[1 - e\sigma(u(z + y) - u(z))](2r - |y|)\chi(2r - |y|),$$

and this suggests the following as a first approximation for the integrated force in (42):

$$-\frac{K}{m}\int_{-h}^{h}[1 - e\sigma(u(z + y) - u(z))](2r - |y|)\chi(2r - |y|)\,dy.$$

However, this does not account for the probabilities of an abutting particle (or bottom) that actually causes the force on a particle centered at z. A reasonable choice is that of a normal distribution that depends on z in a way that the force goes rapidly to zero as $z \to \infty$ having the form

$$\Theta(y, z; b, c) := \frac{1}{b\sqrt{2\pi}}\exp\left(-\frac{((z + y) - b)^2}{2c^2}\right), \tag{44}$$

where a and b are positive constants that can be tuned to match results obtained by simulation or experiment. For the sequel, we choose $b = 7h$ and $c = 3h$. Whence, our IPDE becomes

$$u_t + uu_z = -g - \frac{K}{m}\int_{-h}^{h}\Theta(y, z; 7h, 3h)[1 - e\sigma(u(z + y) - u(z))](2r - |y|)\chi(2r - |y|)\,dy. \tag{45}$$

Again we require auxiliary conditions for well-posedness, and these take the form

$$u(z, 0) = 0, \qquad u(0, t) = \dot{y}_0(t). \tag{46}$$

Once again, it is worth noting that when $e = 0$, (45) represents an infinite-dimensional Hamiltonian dynamical system, inasmuch as it can be written in the form

$$u_t = \theta \circ \nabla H(u), \tag{47}$$

where H is a smooth function, called the Hamiltonian function, ∇ is the standard variational gradient operator for functions and θ is what is called an implectic operator, which plays a role for infinite-dimensional Hamiltonian systems analogous to that of the $2N \times 2N$ matrix

$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix},$$

where I_N is the identity matrix of order N. These notions are all standard in the theory of Hamiltonian dynamical systems, as found in texts such as [Ablowitz and Segur 1981; Arnold 1978; Blackmore et al. $\geq$ 2011; Błaszak 1998; Dickey 1991; Faddeev and Takhtajan 1987; Guckenheimer and Holmes 1983; Katok and Hasselblatt 1995; Prykarpatsky and Mykytiuk 1998], but are a bit too mathematical to delve into here.

Observe that in a manner analogous to that in the L-W formulation above, one also can use the solution $u = (z, t)$ to determine the density via

$$\frac{\partial\rho}{\partial t} + u\frac{\partial\rho}{\partial z} + u_z\rho = 0, \tag{48}$$

subject to the Cauchy data (46).

6. Dynamics of continuum models

If, as indicated by our preliminary study here, the infinite-dimensional dynamical systems in the form of PDEs and IPDEs obtained using the L-W and BSR methods, respectively, provide good approximations to the behavior of a fairly rich variety of granular flows, it follows that we may be able to bring many of the tools of nonlinear dynamics to bear on a multitude of related problems of practical interest. Here we shall only give a couple of examples - in the form of theorems — related to wave propagation in granular media.

First, we consider the L-W approximation (37) and the possible existence of the kind of persistent stable wave structure associated with solitons, which were first described by Zabusky and Kruskal [1965] and have since become an important fixture of the modern theory of dynamical systems, as indicated by such treatments as [Ablowitz and Segur 1981; Blackmore et al. ≥ 2011; Błaszak 1998; Dickey 1991; Faddeev and Takhtajan 1987; Prykarpatsky and Mykytiuk 1998]. And these solitons associated with integrable systems have become increasingly important in applied research in general, and granular flow investigations in particular. Nesterenko [1983] was the first to analytically show the existence of solitons in L-W approximations of a horizontal chain of particles with perfectly elastic Hertzian interactions, which he validated by observing soliton like behavior in actual physical experiments. His equations were obtained by fourth order L-W approximations analogous to (37), except for the gravity term. He showed that his equations can be transformed into the Korteweg–de Vries equation, which is well known to be integrable and so admit soliton solutions. The transformation that he used can be readily modified for our vertical, Walton–Braun rather than Hertzian interactions, to prove the following result.

Theorem 2. *The infinite-dimensional Hamiltonian system* (37) *is integrable when $e = 0$; therefore it admits soliton solutions.*

Several years after Nesterenko's pioneering work on solitons in L-W approximations of one-dimensional Hertzian particle chains, Blackmore and Dave [1997] analyzed approximate models of the same kind of particle chains assuming Walton–Braun particle-particle and particle-wall interactions using the BSR method. They found that a further approximation using the BSR approach yielded Burgers' equation, which is another well-known example of an integrable PDE admitting soliton solutions. The Hamiltonian system obtained from (45) when $e = 0$ is also integrable, and this can be proved by showing that there exists another independent representation of the form (47) satisfying certain assumptions guaranteeing that the system is bi-Hamiltonian (cf. [Błaszak 1998]) in a way that implies integrability. We shall only state this result here, leaving the proof to a forthcoming paper.

Theorem 3. *If $e = 0$, the BSR model* (45) *is an integrable Hamiltonian dynamical system.*

7. Illustrative examples

Here we present examples of a numerical solution of the one-dimensional tapping equations (together with auxiliary data) obtained using both the L-W and BSR methods. In each case we use the simplified hybrid method — described for the L-W model in Section 4 and the BSR model in Section 5. The partial differential operators in equations (37) and (45) are approximated using central differences with equal time and distance steps of 0.01 and the integral in (45) is computed using the trapezoidal approximation.
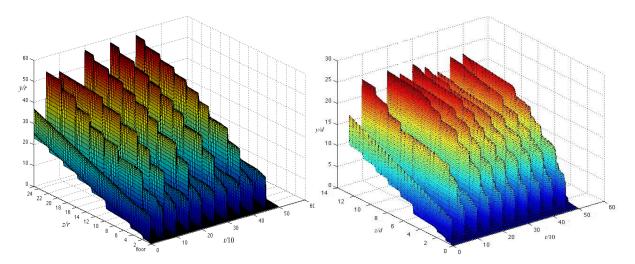
Figure 2. L-W (left) and BSR (right) approximations of tapping solution surface with parameters in Figure 1, right.

We use the same parameters as in the ten-particle example in Figure 1, right, but consider a much longer tap duration, so that we can compare the approximate numerical solutions of the continuum models to the numerical solutions of the exact Newtonian initial value problem (24)–(25).

The solution surfaces of the approximate L-W and BSR solutions are shown in the two halves of Figure 2. One can see that both approximate continuum solutions are very close to one another — both qualitatively and quantitatively — and they show good qualitative agreement with the (numerical) solution of the exact system of ODEs as depicted in Figure 1, right.

8. Concluding remarks and future research

We have shown that both the L-W and BSR approximate continuum models for the one-dimensional tapping problem have solutions that are in rather good qualitative agreement with exact lattice solutions. It seems reasonable to assume then that both of the approximate continuum approaches employed in this paper are viable predictive tools for higher-dimensional and more varied granular flows. Consequently, it just may be that a wealth of useful information can be mined from a dynamical systems oriented investigation of these relatively simple continuum models. With this in mind, we plan, in our future research, to investigate the potential of these infinite-dimensional models using a combined dynamical systems, simulation and visualization approach.

From the dynamical systems perspective, we shall first generalize the two continuum approaches to two- and three-dimensional tapping flows. Extension of the L-W method to two and three dimensions is inherently more difficult than the BSR approximation, because the lattice equations from which it is derived get quite a bit more complicated due to the increasing number of possible regular lattices (square, hexagonal, cubic, tetrahedral and more) to choose from and the increased complexity of nearest-neighbor dynamical equations, as indicated in [Ruiz-Ramírez and Macías-Díaz 2010; Zolotaryuk et al. 2000]. Naturally, we shall have to perfect our numerical treatment of the resulting boundary-initial value problems (which we conveniently simplified using a hybrid method in this paper) in order to validate

the dynamical predictions obtained from the continuum models. And having a rigorously formulated and coded numerical simulation approach will be a must as we extend the continuum approximation approach to additional types of (higher-dimensional) granular flow regimes.

We also expect the nonlinear dynamics approach to be especially useful in detecting and analyzing such phenomena as jamming and force chains. Roughly speaking, jamming can be associated with nearly invariant subregions of the dynamical systems, and force chains can be identified with connected nearly invariant networks in the resulting stress tensor fields. From a more mathematical perspective, we envisage obtaining new theoretical results linking the integrability of the limiting continuum approximations with the integrability of the exact finite systems, possibly yielding new examples of higher-dimensional integrable systems and novel KAM theory type results for systems that are only nearly integrable to begin with (see [Arnold 1978; Katok and Hasselblatt 1995; Kuksin 1993], for example) or results akin to those in [Prykarpatsky et al. 1999] when slight inelasticity renders the dynamics only nearly Hamiltonian.

Our approach using dynamical systems theory is intended to go hand-in-hand with novel refinements and extensions of existing simulation capabilities in a manner that both informs and validates the analysis. One of the applications intended for the models we have discussed in this paper is that of "density relaxation", in which a vessel of granular materials subjected to vibrations or tapping experiences an increase in its bulk density. Because the ability of granular materials to undergo this change in density is an inherent property that is not well-understood, this remains a critical impediment in developing predictive models of flowing bulk solids. We intend to address this issue in future studies by applying the dynamical systems models described in this paper to a system of uniform spheres in an attempt to determine how the various features of the motion scale with the total mass, and the details (e.g., amplitude and frequency) of the floor motion. In particular, our recent stochastic and discrete element findings on density relaxation, reported in [Dybenko et al. 2007; Rosato et al. 2010a; 2010b], have suggested the importance of the tap amplitude in the evolution of granular microstructure, as well as a strong effect of the bulk mass of the system.

An indispensable component of our future research is the kind of sophisticated dynamical systems oriented computer visualization that has come to the fore in recent year in work such as [Haller 2001; Lindeberg 1998; Tricoche et al. 2008]. As our theoretical and computational investigation moves toward more complex, higher-dimensional, and larger-scale granular systems, the interpretation and analysis of our models will become significantly more difficult and require dedicated tools that do not yet exist. We are therefore initiating a research thrust in visual data analysis aimed at supporting the characterization of salient structural and quantitative properties of the systems. Our work will explore an approach connecting the dynamical systems perspective to differential geometric structure definitions. The latter will then form the basis of abstract visual representations that address the visual clutter of large particulate assemblies.

Specifically we will apply a topological framework [Tricoche et al. 2008] to characterize the structural skeleton of the stress field acting upon the system and study its relationship with relaxation and jamming behaviors. Moreover we will study invariant manifolds of the system's dynamics by extending to the discrete setting the notion of Lagrangian coherent structures that has been recently introduced in the nonlinear dynamics and fluid mechanics literature [Haller 2001]. Finally, we will devise a novel scale space framework [Lindeberg 1998] suitable for the detection of salient core and edge manifolds in granular assemblies and explore their relationship with observed physical properties of granular flows.

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