Simulation, modeling and dynamical analysis of multibody flows

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Recent particulate flow research using a discrete element simulation-dynamical systems approach is described. The simulation code used is very efficient and the mathematical model is an integro-partial differential equation. Examples are presented to show the effectiveness of the approach.

Keywords: Newton-Euler equations; DEM simulation; BSR model; reduced models; chaotic dynamics.

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1. Introduction

Granular dynamics has been the focus of intense research for over fifty years now, largely due to the breadth and importance of its applications and the many interesting and challenging engineering and mathematical problems associated with it.
However, although a great deal has been learned about granular flows as a result of the investigations, there remains a plethora of fundamental questions that have not been satisfactorily resolved. This is especially true when it comes to mathematical models capable of predicting a wide range of dynamical phenomena for a broad swath of granular flow regimes. To put it quite simply, there is, for granular flows, nothing like the Navier–Stokes equation, which has proven to be such a reliable dynamical predictor over almost the entire spectrum of fluid flows. Therefore, one must often rely on either experiments or simulations based on classical mechanics to obtain useful information about granular (particulate) flows.

In this paper, we provide a brief but rather detailed account of some of recent results obtained using our combined simulation-dynamical systems approach, which illustrates the efficacy of the method and its potential for extension to dynamical flow field problems of a far more general nature than those of the purely granular type.

The exposition is organized as follows. In Sec. 2, the focus is on the simulation component of the approach. First, Newton’s laws are employed to formulate the equations of motion for configurations comprising large numbers of particles in Euclidean \( n \)-space, where \( n \) can be 1, 2 or 3. Then the basic elements of the discrete element integration algorithm used in our simulation code are described. Next, in Sec. 3, we derive the continuum (BSR) model in a more general setting than that in which it was first introduced. Some of the nice mathematical features of the BSR model are summarized as are various applications investigated in our ongoing research. In Sec. 5, several application examples, primarily for one-dimensional granular flows, are described and comparisons between direct simulations and solutions of the BSR model are discussed. Finally, the results presented are summarized and directions for future related research are indicated.

2. Simulations

In order to provide the context for a description of the discrete element (DEM) simulation code used as well as for the exposition in the sequel, it is necessary to first define some terms, delineate the basic assumptions and posit the equations of motion that mark the starting point of our approach.

Let \( N \) solid spherical particles \( P_1, \ldots, P_N \) with respective radii \( r_1, \ldots, r_N \), small masses \( m_1, \ldots, m_N \) and mass centers \( x_1, \ldots, x_N \) that are assumed to be contained in a region (subset) \( \Omega(t) \) of Euclidean \( n \)-space for all time \( t \geq 0 \). This inclusion and containment is usually denoted as \( x_k \in \Omega(t) \subseteq \mathbb{R}^n \) for all \( 1 \leq k \leq N \) and \( t \geq 0 \), where for most applications it may be assumed that \( 1 \leq n \leq 3 \).

Without further assumptions, the classical equations of motion (including translation and rotation) would be those of Newton–Euler, which are relatively simple for spherical rigid bodies. These equations involve forces that comprise the resultant of both normal and tangential components obtained from the appropriate interaction and external applied force models. The resultant force and moment fields would
then include the physical properties of the particles in the “obvious” way, as exemplified by the force on two disjoint spheres being zero until they collide (neglecting the small gravitational attraction), with the resulting deformation and physical properties, such as their coefficients of restitution mediating the actual force and moment fields.

2.1. Classical equations of motion

With the above assumptions, one starts with the Newton–Euler equations of motion

\[
m_k \ddot{X}_k = F_k(X, \dot{X}, t) + E_k(X, \dot{X}, t),
\]

\[
I_k \dot{\omega}_k = M_k(X, \dot{X}, t) + L_k(X, \dot{X}, t), \quad (1 \leq k \leq N)
\]

where a dot over a variable denotes the time derivative \(d/dt\), \(X := (x_1, \ldots, x_N)\) is the \(nN\)-dimensional vector associated to the configuration space of Eq. (1), \(\omega := (\omega_1, \ldots, \omega_N)\) is the angular velocity vector with components the angular velocities about the centers of mass of the corresponding spheres, \(F := (F_1, \ldots, F_k)\) and \(M := (M_1, \ldots, M_N)\) are, respectively, the particle–particle and particle–boundary (\(\partial \Omega(t)\)) interaction force and moment fields, and the last terms on the right-hand sides are the \(k\)th components of the external force and moment fields, respectively, on the particle configuration; namely, \(E := (E_1, \ldots, E_N)\) and \(L := (L_1, \ldots, L_N)\), which are usually just due to gravity, but may include electromagnetic and other forces and moments. Note that our assumption on the containment of the particles can be succinctly denoted mathematically as follows: The solution \(x = x(t) \in \Omega(t) \times \cdots \times \Omega(t) := \Omega(t)^N\) for all \(t \geq 0\).

2.2. Simulation details

Equation (1) in space \((n = 3)\) can, in the usual fashion, be recast as a system on \(9N\) first order ordinary differential equations for the positions of the particles and their angular velocities. Naturally, this is a system that can be solved numerically by a standard Runge–Kutta method, possibly with variable step sizes. There is however a numerical problem with the interaction forces that are typically used. For our code, the Walton–Braun dissipative normal force model\(^3,4\) is used, which upon contact is based on a linear spring \((K_1)\) for compression or loading and another stronger linear spring \((K_2)\) for expansion or unloading. There is also a tangential frictional force based on the Mindlin–Deresiewicz model,\(^5\) and the combination of the two has been used in numerous investigations.\(^6–8\) These interaction model choices, as well as most of those chosen in the literature, render the system (1) very stiff; so much so in fact, that the use of one-step solvers becomes problematical when it comes to computational efficiency.

One could try multistep or predictor–corrector methods to ameliorate the stiffness problem in numerically integrating Eq. (1), but we have found that the discrete element Verlet–Störmer leapfrog numerical integrator\(^9,10\) is the most effective and
efficient tool for our granular dynamics code. This integrator works as follows: Let-
ing a superscript \( i \) denote the time-step value in the leapfrog difference scheme,
one computes the update of the position \( x^i \) using the finite difference equations
\[
\dot{x}^{(i+1/2)} = \dot{x}^{(i-1/2)} + \omega^{(i+1/2)} = \omega^{(i-1/2)} + \omega^{(i)} \Delta t, \tag{2}
\]
and then calculates the updated position as
\[
x^{(i+1)} = x^{(i)} + \dot{x}^{(i+1/2)} \Delta t. \tag{3}
\]

3. Modeling and Analysis

We begin this section with a derivation of a generalized version of the BSR model: a continuum integro-partial differential equation (IPDE) first intro-
duced as a possible relatively simple governing equation for a variety of granu-
lar flows, which enjoys the rather unusual property of being directly amenable to
rigorous mathematical analysis.

In pointing to some of the outstanding features of the BSR model, we are by
no means discounting the extensive and impressive research done on creating and
analyzing such simplified models, which has advanced our knowledge of granu-
lar flows considerably over the last few decades. Some — just a few — notable
examples of these efforts are the continuum models obtained either from first prin-
ciple, modifications of the Navier–Stokes equations or various continuum limits
such as in Bougie et al., Farrel et al., Goldshein and Shapiro, Hayakawa and
Hong, Hennan and Kamrin, Jenkins and Savage, Jenkins and Richman, Nesterenko,
Pitman, Rajagopal, Savage, Schaeffer, Schaeffer et al., and Wakou et al. as well as
those using lattice dynamics or related methods such as in Freisecke and Wattis,
MacKay, Sen and Manciu, Baxter and Behringer and Caram and Hong.

3.1. The generalized BSR model

The generalized BSR model shall now, in the interest of simplicity, be described in
Euclidean \( n \)-space, although it should be noted that it could be readily modified
to suit curved spaces or manifolds. Once again, it is assumed that the particle
configuration is contained in a region \( \Omega(t) \) in \( \mathbb{R}^n \) for all time \( t \geq 0 \).
However; in this case, the object is to apply a continuum limit that produces an IPDE. There
are, of course, direct contact particle–particle and particle–boundary interaction
forces, but in contrast to the original BSR model, possible forces at a distance,
for example in the case of magnetized particles, are also considered.

In Euclidean \( n \)-space, the generalized BSR model, comprising a momentum and
continuity equation, has the form
\[
u_t + (u, \nabla) u = e(x, t) + \int_{R(x)} \rho(y, t) \Theta(x, y, t, u(x, t), u(y, t)) dy,
\]
\[
\rho_t + (u, \nabla) \rho = -\rho \text{div } u = -\rho \text{tr } u_x = -(\partial_x u + \cdots + \partial_{x_n} u) \rho,
\]
which is subject to the $C^2$ Cauchy initial data
\[ u(x, 0) = \varphi(x), \quad \rho(x, 0) = \psi(x), \quad (x := (x_1, \ldots, x_n) \in \mathbb{R}^n) \quad (6) \]
and is to be solved on $\Lambda := \{(x, t) \in \mathbb{R}^{n+1} : 0 \leq t, x \in \Omega(t) \subset \mathbb{R}^n\}$, where $t \to \Omega(t)$ is a $C^2$ map into the space of subsets of $n$-space with piecewise $C^2$ boundaries. In the above equations, $u = u(x, t) := \dot{x} = (\dot{x}_1, \ldots, \dot{x}_n)$ is the velocity, $\rho = \rho(x, t)$ is the density, $e$ is the external force per unit mass, if any, $R(x)$ is the subset of $n$-space containing $x$, called the region of influence on $x$, in which the particle at this point is acted upon forces by direct particle–particle or particle–boundary interactions and forces at a distance, should there be any, and $\Theta$ is the force per unit mass kernel (per unit mass$^2$) that represents all of the internal interaction forces in the sense that $\rho(x, t)\Theta(x, y, t, u(x, t), u(y, t))$ is the interaction force per unit mass per unit volume at $x$ generated by the mass at $y$.

3.2. Derivation of the model

What follows is a derivation of the model wherein, in the interest of brevity, some of the routine details are left to the reader. The analysis follows a point particle moving through the dynamical domain $\Omega(t)$ as shown in Fig. 1.

Using the discrete particle notation in Sec. 1 in conjunction with the definitions associated to Eqs. (3) and (4) together with the usual transport equations for trajectory dynamics,$^{33}$ we obtain the combined continuum–discrete momentum equation
\[ \rho(x, t) \frac{D u}{Dt} = \rho(x, t)(u_t + \langle u, \nabla u \rangle) \]
\[ = \rho(x, t)e + \sum_{k=1}^{N(x)} \rho(x, t)\Theta(x, y_k, t, u(x, t), u(y_k, t))\Delta y_k, \quad (7) \]

Fig. 1. (Color online) An illustration of the transport based derivation of the BSR model for a flow field configuration in a compact region with a smooth boundary in Euclidean 2-space.
where \( N(x) \) is the number of particles (including points on the boundary of the dynamical domain) that interact with the particle \( x \) by direct collision or at a distance.

Then, letting the number of particles go to infinity, with the corresponding increments \( \Delta y \) going to zero, the summation converges to an integral and yields the momentum equation (4) of the BSR model, which when combined with the continuity equation (5) comprises the complete system with the usual type auxiliary data and specification of the dynamical domain provided by Eq. (6) and the definition of \( \Lambda \).

3.3. Analysis of the model

The relative simplicity of the BSR model renders it more amenable to mathematical analysis than most of the other continuum models used these days. In fact, we can prove global well-posedness of the system (4)–(6) under very reasonable assumptions, which appears to be a first for any such models. In particular, Wu proved, using an innovative method of characteristics-based approach, the following result in his dissertation.\(^{34}\)

**Theorem 1.** Let the BSR system (4)–(6) be \( C^2 \) and satisfy the a priori estimate: \( \rho \) is bounded on \( \Lambda \). Then the system has a unique \( C^1 \) solution on \( \Lambda \) that depends continuously on the initial Cauchy data (6).

Another of the analytical properties for the BSR model is along the lines of the complete integrability results proved by Nesterenko\(^{20}\) for long-wavelength continuum limits of one-dimensional particle configurations with Hertzian interaction forces. Namely, Blackmore et al.\(^{35}\) proved the following result using Magi’s theorem\(^{36}\) for bi-Hamiltonian infinite-dimensional Hamiltonian dynamical systems.

**Theorem 2.** Suppose Eq. (4) represents a one-dimensional model for the dynamics of a system of particles with no external force and perfectly elastic direct interaction forces. Then it is a bi-Hamiltonian dynamical system, which is completely integrable in the sense that it has an infinite sequence (hierarchy) of independent, mutually involutive invariants.

3.4. Numerical analysis of the model

In addition to the analytical results that Hao obtained in his thesis, he developed a very effective and efficient semi-discrete numerical integration scheme for the BSR model, which employed central finite differences in space and a third-order Runge–Kutta integrator for time (see Rosato et al.\(^{8}\) for details). Moreover, he was able to show, using the elements of the proof of Theorem 1, that the scheme is consistent, convergent, stable, and is second-order accurate in all variables.

For the one-dimensional problem in which a column of inelastic spheres (of diameter \( d \)) is subjected to sinusoidal taps, our model (4)–(6) for the velocity \( u \) and
density $\rho$ takes the form

$$ u_t + uu_y = \frac{1}{mm_o} \int_{-2r}^{2r} F(\rho)dz - g + a\omega^2 \sin \omega t, $$

$$ F(\rho) := K_1 \rho(y+z,t)(2r - |z|)\sigma(z)(1 - e\sigma(z[u(y-z) - u(y)])), $$

$$ \rho_t + u\rho_y = -\rho u_y, $$

$$ u(y, t = 0) = 0, $$

$$ \rho(y, t = 0) = \rho_0(y), $$

where $a\omega^2 \sin \omega t$ is the external force per unit mass, $g$ is gravitational acceleration, $K_1$ is the loading stiffness in the Walton–Braun model,

$$ m = \frac{4\pi \rho d^3}{3}, \quad \sigma(s) := \begin{cases} 1, & s > 0 \\ 0, & s = 0 \\ -1, & s < 0 \end{cases} $$

and $m_o$ is a characteristic mass. Note that (8) contains only a single fitting parameter, namely $m_o$, which arises from the reduction of the full three-dimensional model (4)–(6). The result of the numerical scheme used to solve (8) is illustrated in Fig. 2, which shows trajectories of a tapped vertical column of identical particles $e = 0.9$.

### 3.5. Reduced models

The BSR model, possibly in conjunction with the classical equations of motion, can under certain simplifying assumptions be used to obtain reduced models that reveal various important aspects of the dynamics. In some cases, the reduced models can be much simpler and considerably more amenable to detailed analysis. For example, Blackmore et al.\textsuperscript{37} prove that the motion of the center-of-mass of a periodically...
tapped column of (a large number of) particles can be approximated quite well by the iterates of a smooth \((C^\infty)\) planar transformation

\[ F : \mathbb{R}^2 \rightarrow \mathbb{R}^2, \tag{9} \]

of the standard map type used by Holmes\(^{38}\) to model the motion of a single particle bouncing on an oscillating plate.

This map was then proved, using some results of Joshi and Blackmore,\(^{39}\) to have very complex dynamics for sufficiently vigorous periodic tapping of a column of particles. This result, summarized in the following theorem, is an indicator of similar dynamic behavior of the entire particle configuration.

**Theorem 3.** If the product of the amplitude and impact speed of the periodic taps of the vertical column center-of-mass modeled by the map (9) is sufficiently large, the discrete dynamical system comprising the iterates of \(F\) has a chaotic strange attractor, which plausibly implies the same for the entire system.

### 4. Examples and Applications

This section is devoted mainly to illustrating the DEM simulation code and the semi-discrete numerical scheme for the BSR equations for one-dimensional granular flows, with an eye toward comparing these two methods for describing the dynamics. A number of the more obvious applications shall be touched upon as well as a rather new one describing possible employment of magnetized particulates, which is part of our current research.

#### 4.1. One-dimensional granular dynamics

In what follows, a description of several comparisons of the DEM and semi-discrete numerical solutions of problems related to tapping granular columns are presented, along with details of the system geometry and interaction model. Naturally, we make use of the form of the BSR model (4)–(6) for this one-dimensional case given by Eq. (8), which is numerically integrated (as described in Sec. 3.4).

The coordinate system is such that sphere centers \(\{y_k(t), k = 0, 1, 2, \ldots, N\}\) are initially positioned at \(\{y_k(t), k = 0, 1, 2, \ldots, N\}\), while gravity points in the \(y\)-direction.

The \(N\) identical spheres of diameter \(d\) are constrained by integrating their equations of motion via (2) and (3) only in the vertical direction so that their centers remain aligned. The absence of bounding side walls precludes rotations of the spheres through friction-induced tangential momentum transfer. Applied to the floor is a half-sine pulse given by

\[ y_0(t) = \begin{cases} 
  a \sin(\pi t / \tau), & 0 \leq t \leq 1/\tau, \\
  0, & 1/\tau \leq t, 
\end{cases} \]

where \(\tau = 1/2f\) is the period and \(f\) is the frequency. The integration time-step is first estimated by the loading period \(e \sqrt{\rho \pi d^3 / 12K_1}\), and then reduced so that no
overlap between contacting spheres exceeds 1% of the diameter \( d \). This configuration is shown in Fig. 3.

Several comparisons of the tapping dynamics predicted by simulation and the semi-discrete integration scheme, comprising central difference approximations in space and third-order Runge–Kutta integration in time, shall be presented. The cases considered are those with columns of 10 or 20 identical spheres, all with diameter \( d = 0.2 \) cm and coefficient of restitution \( e = 0.9 \) or 0.98. Both single and multiple (periodic) taps are considered, with the tap duration \( \tau = 0.05 \) s in each case. Tap amplitudes are always either \( a = 0.75d \) or \( a = d \), and the frequency of multiple tapping is chosen to be 10 Hz.

![Fig. 3. (Color online) Tapping of vertical column of identical spheres.](image)

\[
y_0(t) = \begin{cases} 
  \alpha \sin(\omega t), & 0 \leq t \leq \pi/\omega \\
  0, & \pi/\omega \leq t \leq T 
\end{cases}
\]

\( \tau_r = 0 \) Continuous vibration

\( \tau_r \) Time interval between taps

Fig. 4. Comparison of dynamics for a single vertical tap at \( t = 0 \) of a 10-ball column with \( a = d \) and \( e = 0.98 \), with the ten center trajectories plotted using the BSR model. The dotted curve just above the time-axis is a plot of \( S \) as defined by Eq. (10).

![Fig. 4.](image)
Fig. 5. Comparison of dynamics for periodic vertical tapping starting at $t = 0.4$ sec of a 20-ball column with $a = 0.75d$ and $e = 0.9$, with the center trajectories plotted via simulation. The thicker curve just above the time-axis is a plot of $S$ defined by Eq. (10). Arrows along the time-axis indicate periodic taps.

Fig. 6. (Color online) Comparison of normalized kinetic energy ($KE_n := KE/KE_{max}$) for a single vertical tap at $t = 0.4$ s of a 20-ball column with $a = d$ and $e = 0.9$. The continuous curve represents the results of simulation, while the thicker dashed curve is obtained from numerical solution of the system (8).

Figure 4 shows the comparison for a ten sphere single-tap system, with a plot of the sphere center trajectories obtained by numerical solution of system (8) on which is superposed a plot of the maximum separation of the these and the simulated trajectories. More precisely, the separation plot is the graph of

$$S(t) := \max\{|\tilde{y}_i(t) - \hat{y}_i(t)| : 1 \leq i \leq N\},$$

(10)

where $\tilde{y}_i$ and $\hat{y}_i$ are, respectively, the numerically computed BSR and simulated trajectories of the $i$th sphere center.

For our next comparison, we consider the periodic tapping of an $N = 20$-ball column illustrated in Fig. 5.
For the final comparison shown in Fig. 6, we consider a single tap applied at \( t = 0.4 \) to a 20-ball column, and compare the total kinetic energy of the system as computed via simulation and numerical solution of Eq. (8).

The comparisons between simulation solutions and numerical integration of the BSR model show very good agreement, with the largest differences being of order 0.01\( d \). Note also that, as one might expect, the largest difference tend to occur when the lower portion of the configuration changes direction after interacting with the floor.

### 4.2. One-dimensional magnetized granular flows

The motion of one-dimensional arrays of magnetized particles appear to exhibit very interesting properties, some of which indicate they may have important applications in areas such as energy harvesting.

A new direction in our research, reported by Blackmore et al.,\(^40\) involving magnetized particle dynamics, shall be described very briefly in what follows. Various applications of such research have already been studied by several authors (see e.g., Manciu et al.\(^41\)). Assume that the magnetic material is continuously distributed along a line, but concentrated in finitely many small intervals identified as point magnets at the interval midpoints. Integration of the \( 1/r^2 \) forces over the intervals produces \( 1/r \) interaction forces among the point magnets. Let \( N \) point magnets of masses \( m_1, \ldots, m_N \) and strengths per unit mass \( \gamma_1, \ldots, \gamma_N \) lie along \( \mathbb{P} \) at the points \( x_1, \ldots, x_N \). The Hamiltonian equations of motion with \( 1/r \) interaction forces are

\[
\dot{x}_k = \{H_0, x_k\}, \quad \dot{y}_k = \{H_0, y_k\} \quad (1 \leq k \leq N),
\]

where the momenta \( y_k \), Hamiltonian function \( H_0 \) and (nonstandard) Poisson bracket \( \{\cdot, \cdot\} \) are defined, respectively, as

\[
y_k := \dot{x}_k, \quad H_0 := (1/2) \sum_{k=1}^{N} \gamma_k y_k^2 - \sum_{1 \leq j < k < N} \gamma_j \gamma_k \log |x_j - x_k|,
\]

\[
\{f, g\} := \sum_{k=1}^{N} \gamma_k^{-1} \left\{ f_{y_k} g_{x_k} - f_{x_k} g_{y_k} \right\}.
\]

For point magnets in Euclidean \( n \)-space \( \mathbb{R}^n \), the equations of motion are the analogous. If one omits the kinetic energy in \( H_0 \), it is of the form of the Hamiltonian for point vortices in an ideal fluid.

On the other hand, if one retains the kinetic energy term, it can be identified with the precession velocity in the point vortex equations for the approximate quasi-2D model\(^42\) of Bose–Einstein condensates (BEC); namely,

\[
\gamma_k \ddot{z}_k = -2i\gamma_k \partial_{\bar{z}_k} \Phi(z) - i \sum_{1 \leq j \neq k \leq n} \gamma_j \gamma_k (\bar{z}_j - \bar{z}_k)^{-1} \quad (1 \leq k \leq N),
\]

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where \( z_k = x_k + iy_k \in \mathbb{C} \), the complex plane, and the leading term on the right-hand side is the component of the precession velocity. Note that the system (12) is also Hamiltonian, with Poisson bracket as above and Hamiltonian function

\[
H = \Phi(z) - \sum_{1 \leq j < k \leq N} \gamma_j \gamma_k \log |z_j - z_k|.
\]  

(13)

This interesting connection between the dynamics of the system (11) and BEC vortices suggests that vorticity may play an important role in magnetized granular flows.

5. Conclusions and Related Future Research

We have shown how sophisticated DEM simulations in concert with the BSR model provide powerful tools for the investigation of granular flows of inert particles, and indicated how they can also be used to analyze and predict the dynamics of particulates with intrinsic force fields, such as those of electromagnetic type. Considerable work remains to be done in several areas, including enhancing the DEM code to include a wider range of interaction forces and extending and improving the numerical solution scheme for the BSR model. These types of extensions and improvements are the focus of our current research on granular flows in which we are starting with 1-dimensional configurations, with the intention of ultimately being able to handle very general 3-dimensional flows. We are also developing experimental procedures to enlighten and confirm the simulation and dynamical system aspects of the research. Lastly, we shall continue to seek significant applications of our results, especially for particulates with intrinsic force fields, where it appears that there are some promising opportunities in the realm of applied energy research.

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