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Numerical modelling of granular flows: a reality check

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Abstract Discrete particle simulations provide a powerful tool for the advancement of our understanding of granular media, and the development and refinement of the multitudinous techniques used to handle and process these ubiquitous materials. However, in order to ensure that this tool can be successfully utilised in a meaningful and reliable manner, it is of paramount importance that we fully understand the degree to which numerical models can be trusted to accurately and quantitatively recreate and predict the behaviours of the real-world systems they are designed to emulate. Due to the complexity and diverse variety of physical states and dynamical behaviours exhibited by granular media, a simulation algorithm capable of closely reproducing the behaviours of a given system may be entirely unsuitable for other systems with different physical properties, or even similar systems exposed to differing control parameters. In this paper, we focus on two widely used forms of granular flow, for which discrete particle simulations are shown to provide a full, quantitative replication of the behaviours of real industrial and experimental systems. We identify also situations for which quantitative agreement may fail are identified, but important general, qualitative trends are still recreated, as well as cases for which computational models are entirely unsuitable. By assembling this information into a single document, we hope not only to provide researchers with a useful point of reference when designing and executing future studies, but also to equip those involved in the design of simulation algorithms with a clear picture of the current strengths and shortcomings of contemporary models, and hence an improved knowledge of the most valuable areas on which to focus their work.

Keywords Granular · Discrete particle method (DPM) · Discrete element method (DEM) · Vibrated · Chute flow · Review

1 Introduction

1.1 Background and aims

Granular materials—assemblies of multiple, discrete particles or 'grains'—are, after water, the second most manipulated material on the planet [1], playing important rôles in multitudinous natural and industrial processes [2–9]. Yet in spite of their ubiquity and industrial relevance, and despite the significant volume of research in the field [10], the behaviours of granular materials remain poorly understood and difficult to predict [11].

Our inability to accurately predict and control the behaviours of granular flows carries many negative consequences for industries required to handle particulate media. For instance, phenomena such as jamming, agglomerating or clogging [12] may significantly reduce the efficiency of industrial flows [13] or even cause catastrophic structural failures in storage silos [14,15]; phenomena such as segregation (gradual separation of dissimilar particle species) [16,17], meanwhile, can prove similarly problematic, for instance

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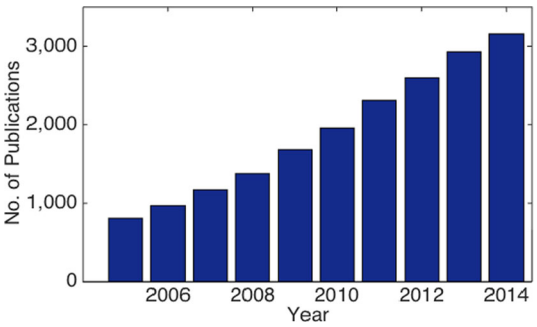

Fig. 1 Illustrates the exponentially increasing research interests concerning discrete particle simulations of particulate systems in the last 10 years. The statistics are obtained from Google scholar using the following keywords: 'discrete element method', or 'discrete particle simulation'

in the pharmaceutical industry [18] where a lack of mixing may—for obvious reasons—have serious repercussions.

In order to avoid issues such as those described above, companies often resort to ad hoc solutions, such as the construction of scaled-down test systems or pilot plants, or even opting to 'hit and hope'—simply constructing a system and attempting to resolve any issues later. The former solution can often prove extremely costly and, since the scaling behaviours of granular materials are also incompletely understood [3,19,20], may still not provide any information relevant to the full-scale setup. The latter, meanwhile, is likely to result in decidedly sub-optimal efficiency or, worse, might fail entirely.

Increasingly, industries are turning away from such 'practical' methods, choosing instead to utilise *computational models*. In particular, simulations produced via the discrete particle method (DPM) [21–29]—or discrete *element* method (DEM) as it is more commonly often referred to—are used in order to gain an understanding and predictive, quantitative knowledge of the dynamical and physical properties of granular systems. Discrete particle models—a rapidly evolving field of research, see Fig. 1—carry a significant advantage over practical investigations (experiments) in that they can provide a *plethora of information* regarding the dynamics of *each particle within the system* at any given point in time. This level of detail is, at present, near-impossible to achieve in practical, experimental settings—techniques which can capture information regarding all particles within a system typically suffer from poor time resolution [30], while systems capable of imaging in real-time can generally only image relatively small systems, or limited fractions of larger systems [31–33]. Similarly, techniques which provide detailed information regarding the *dynamics* of a system [34] are often limited in their ability to provide information regarding detailed structural and contact properties, and vice-versa.

Unfortunately, discrete element methods also carry certain notable disadvantages. Firstly, the simulation of systems containing large ($\gtrsim 10^6$) numbers of particles will typically require hardware which may be prohibitively expensive and timescales which are often unfeasible. Despite the current trends of increasing processing power in computational systems and the falling cost of technology, such a problem is likely to persist for a considerable period of time. This being the case, a more time-efficient alternative is to use discrete element methods only when necessary, i.e. to determine the closure or constitutive relations necessary for a continuum approach (micro-macro mapping— see [35,36] and references therein). Alternatively, it is possible to couple simulations with continuum methods (coupled multi-scale methods, CMSM—see [37–39]).

An additional disadvantage of the discrete element method is the necessity to implement certain modelling assumptions when emulating particulate systems, e.g. particle shapes (spherical or non-spherical), types of interactions (contact models) etc. which are often approximations compared to 'real life'. This raises an important question:

How accurately can DEM models emulate 'real' granular systems?

It is this question which forms the central theme of this paper. The ability of DEM simulations to faithfully recreate the behaviours of physical systems is pivotal to their use as viable predictive models. While we have focussed thus far on the relevance of DEM simulations in *industrial settings* in order to quickly and simply give a feel for the magnitude of the issues at hand, computational models also have numerous other highly important applications regarding questions of science and progress in other disciplines. For instance, granular systems provide useful, easily accessible analogues for various biological systems [40,41] which may be difficult to study in the field, allowing us to extract valuable information regarding, for instance, the behaviours of bacteria [42], animals [43,44] and even humans [45–47]. Computer models of granular systems may even eventually provide us with the ability to predict and prevent disastrous geophysical events such as earthquakes, avalanches and landslides [48–50].

Before any of the above are to be achieved, we must first ensure that computational particle simulations can indeed provide an accurate representation of the real systems which they are designed to represent. In this work we raise, and aim to resolve, a series of questions pertaining to this matter: what is the current state of the field of discrete element modelling? Under what conditions, and for what parameter ranges, can specific systems be accurately modelled at present? How do we ensure that we implement sensible values for particle properties? How can we test the validity of the numerous simplifying assumptions used in simulations? Through an analysis of the existing literature and with reference to our own experimental and numerical work we aim to address these vital and pressing questions.

1.2 Article outline

This article is structured as follows: In the following (Sect. 2), we begin by briefly listing the latest developments relating to the methods used to simulate particulate systems, with particular emphasis on the post-processing techniques implemented. We also detail current works pertaining to parallelised discrete element simulations (Sect. 2.1.1) and micro-macro mapping techniques (Sect. 2.2). We then discuss how discrete element simulations are used in conjunction with experimental systems (Sect. 3), detailing the typical process by which suitable parameters are determined to recreate the real-world system being modelled. We then assess how well DEM results compare to experimental data for two common experimental setups—vibrated beds (Sect. 3.1.1) and inclined channels (Sect. 3.1.2)—and a variety of system parameters. Finally, we summarise our results (Sect. 4).

2 Particle simulations

Over the past decades, a range of computational methods have been developed to address and understand granular dynamics [51]. These include cellular automata (CA), direct simulation Monte Carlo (DSMC), contact dynamics (CD) and the discrete element/particle method (DEM/DPM).

In a simple, deterministic technique such as lattice-based CA, particle positions are determined using rule-based mathematics or physics-based equations determined through experiments. CA utilises a lattice-like structure (grid) in which the physical domain is divided into cells. Each cell corresponds to one of the defined number of states (see Goles et al. [52]). The technique has been used, previously, to understand the flow of granular materials in silos [53–55], in sand piles [52,56], in annular shear cells [57,58], a well as over inclined channels [59,60], in rotating drums [61,62], in hopper flows with irregular particle shapes [63]. Although the method is computationally fast, the predicted particle dynamics lack quantitative accuracy, agreeing only qualitatively with experimental observations.

Granular dynamics have also been modelled using a *stochastic* DSMC approach. This method solves the Boltzmann equation based on direct statistical simulation of the molecular processes described by the kinetic theory, see [64,65]. The technique, first proposed by Bird [64], is both computationally efficient and relatively simple to implement as compared to DEM implementation. The method has been successfully utilised to simulate dilute granular flows in two- and three-dimensional vibrated containers [66] and Couette flows [67], for instance. Recently, modified DSMC algorithms have been developed [68–70] which are faster than traditional DSMC methods and, more importantly, consistent with DEM results [70].

2.1 Discrete element method (DEM)

With the advent of computing technology, research in granular media has literally quadrupled since the past few decades. It was in the late 1970's, when the myth of tracing the trajectory of a particle or grain metamorphosed into a much needed reality. Since then, particle tracking has become essential in numerous applications involving particulate media.

DEM is categorised into two main varieties—hard- and soft-particle [21,51,71]. In the hard-particle (rigid particles) approach, collisions are assumed to be instantaneous and binary, whereas in the soft-particle approach the collisions are considered to be enduring, i.e. the contact duration is finite.[1] Hard-particle-based computations are significantly faster as compared to equivalent soft-particle simulations. Even today, when necessary, studies utilise the hard-particle-based particle simulations, e.g. in dilute collisional flows. However, for dense flows, where particle contacts are enduring and multiple, the soft-particle approach is, clearly, preferable. For a detailed review of these approaches, their corresponding algorithms, theoretical advances and applications refer to recent reviews [21,51,72–74] and the references therein.

Even though majority of the references listed in these articles [21,51,72–74] consider spherically shaped particles, particulate systems encountered in industry or nature are often made up of non-spherical and/or irregularly shaped particles. Studies have shown that particle geometry considerably affects the bulk dynamics of particulate mixtures. As a result, a variety of techniques have been formulated to construct different particle shapes (ellipses/ellipsoids, superquadrics, polygons/polyhedrons, multi-spheres etc.) and to perform efficient contact detection for these more complex geometries. However, we do not review these state-of-the-art techniques as these have already been comprehensively addressed [71,72,75–80].

2.1.1 Computational speedup

Despite tremendous efforts to allow DEM to successfully emulate reality, the computational time associated with soft-sphere DEM has always been considered a liability. While soft-sphere-based DEM provides us with a plethora of useful particle data, these data require a considerable amount of time to compute. For example, let us consider a DEM simulation of a granular mixture. During the simulation process, it is necessary to store and update the particle positions at every time step. The computer must also detect all collisions or contacts between particles and calculate the resulting forces due to these contacts. However, in the case of static mixtures,

[1] Note that particles are geometrically still rigid. However, deformations are taken into account in force models.

e.g. simulations concerning stationary assemblies of rocks, it is the force computations that consume more time because of the fixed neighbours implying contact detection is just a one-time operation. Nevertheless, both contact detection and force computations carry a high computational cost.

As a stepping stone towards minimising this computational effort, recent studies have succeeded in initiating efficient solutions either by developing state-of-the-art contact detection algorithms [81–84] or utilising multi-core [85–87] processors, heterogeneous CPU[2]-GPU[3] architecture [87–90], supercomputers [91] or parallelised GPU clusters [92]. A modern day personal desktop—possessing two or four cores—is able to simulate, for example, two-minute-long, fully three-dimensional simple soft-sphere (linear force model) DEM simulation comprising 10,000–200,000 particles within a couple of hours. A highly parallelised cluster [93–96], meanwhile, would only require a couple of minutes to perform such a task. Despite of advances in parallelised DEM packages, simulation of current industrial applications which involve multitudes of highly polydisperse particles, in the order of 10^9, is difficult because of the inherited complexity in the detection of contacts [86]. As a result, studies have been focussing on a GPU-based framework for developing a highly parallelised GPU-based DEM solver. See [92] for a brief performance overview for CPU- and GPU-based systems.

With such massive parallelism now available using programmable GPU hardware, rapid advancements have been witnessed in the past 10 years. Innovatory simulations on the order of millions of particles are being simulated in quasi real-time in confined environments [97], rotating drums [98], blenders [99] and granular soils [100], to give but a few examples. This is thanks to the sophisticated algorithms developed for efficient collision detection [84,101–107] and the construction of memory-efficient data structure [108]. Using high performance GPU, [109] investigated the size effects in granular mixture flows, whereas [110] used it to simulate fractures in heterogeneous media. Additionally, to bridge the gap between ideal and realistic mixtures, studies have also considered the simulation of non-spherical particles using the GPU-based framework, see [111] for triangular particles, or [112,113] for convex polyhedrals.

2.2 Micro-macro transition

Given that DEM is an efficient tool utilised to probe the intricate details of granular dynamics, macroscopic quantities such as density, velocity, stresses and other necessary fields are essential in any analysis involving validation or calibration of a continuum model. Besides using this mapping tool to calibrate or validate continuum models, macroscopic fields are useful to quantitatively compare experiments and particle simulations as well. For example, let us consider monodisperse flows (mixtures made up of particles of the same type) over inclined channels. In these experiments, often techniques such as particle image velocimetry [115] are used to obtain velocity fields [116]. In order to compare these fields with the DEM simulations, a micro-macro technique is essential.

Mapping of the microscopic scale dynamics onto a macroscopic scale, e.g. continuum, has been under focus since the classical studies by [117,118] and others [119]. Based on a variety of theoretical postulates, various methods for local averaging have been formulated to extract these macroscopic quantities efficiently, for instance the binning of the microscopic fields into small volumes [73] and the method of planes [120]. However, most methods are restricted in terms of their application due to various limitations, (see [73] and the references therein). One of the requirements for multi-scale methods is to efficiently map the particle dynamics (microscopic) onto a macroscopic field which in turn satisfy the classical equations of continuum mechanics, i.e. the fundamental balance law of mass and momentum

$$\begin{aligned} &D(\rho) + \rho\nabla\cdot\mathbf{u} = 0,\\ &D(\rho\mathbf{u}) + \rho\mathbf{u}\nabla\cdot\mathbf{u} = \nabla\cdot\boldsymbol{\sigma} + \rho\mathbf{g}. \end{aligned} \tag{1}$$

The above equations are stated in terms of mass density ρ, bulk velocity $\mathbf{u}$ and the stress tensor $\boldsymbol{\sigma}$. Coarse graining[4] approaches to granular materials first appeared in the work of [121] and has been extended by a number of studies [122–133]. Coarse-graining techniques have two essential advantages over other types of averaging techniques. Firstly, the macroscopic quantities produced exactly satisfy the continuum laws of motion. Secondly, they are applicable to both static and dynamic granular media. With these advantages, the coarse-graining approach has been utilised to study the results of computations or experiments and characterise them in terms of their density, velocity, stress, strain, couple-stress and other fields [134–140]. Futhermore, the coarse-graining method described in [133] has been extended to granular mixture flows near boundaries or discontinuities [141,142] and bidisperse mixtures [36,143]. These extensions [141,143] have been applied to analyse layered flows [35,144] and segregation phenomena in bidiserpse granular mixtures [36].

[2] Central processing unit

[3] Graphics processing unit

[4] On a different note, in molecular dynamics, the same term coarse graining is used when a system is represented by a reduced (in comparison with an all-atom description) number of degrees of freedom. Due to the reduction in the degrees of freedom and elimination of fine interaction details, the simulation of a coarse-grained (CG) system requires less resources and goes faster than that for the same system in all-atom representation. As a result, an increase of orders of magnitude in the simulated time and length scales can be achieved.

3 Discrete particle simulations and experimental systems

Even with the innovatory theoretical extensions discussed in Sects. 2.1 and 2.2, emulations of 'real' particulate systems or experiments is still non-trivial. Figure 2 illustrates two conceivable modelling philosophies which utilise discrete element simulations. In Fig. 2a, we see a conventional approach adopted by the majority of contemporary studies dealing with validation and calibration of discrete element simulations using experiments. Single particle experiments are vital for establishing the contact parameters (material properties) essential in discrete element simulations. Once appropriate values for the contact parameters are established, both small- and large-scale simulations are set up. Through small-scale simulations, one is able to understand the intricate dynamics—by micro-macro mapping—essential for developing an accurate predictive continuum model. Once the continuum model is formulated, it can then be validated using a large-scale simulation or experiments. There exist several granular continuum formulations which need closure or constitutive relations which are unknown, e.g. [145–147], and need to be determined experimentally or via DEM simulations, e.g. [35,36,148]. However, when modelling more complex particulate systems, a two-way coupled multi-scale mechanics (CMSM) approach is adopted, see Fig. 2b. Single particle experiments are utilised to determine the particles' material properties which in turn are incorporated into small-scale discrete element simulations. With the right material parameters, the two simulation models (DEM and continuum) are dynamically coupled such that a two-way feedback exists between the two models. The idea is to use a macroscopic continuum model even where the continuum method fails. In this case, the microscopic model, i.e. DEM, solves for the non-continuum part locally and constructs meaningful macroscopic data which is incorporated into the continuum model. The coupling is performed in select regions in space and time, thus reducing the computational expense and allowing for the simulation of complex particulate systems. A detailed review of this method is given by Weinan et al. [37].

Continuum theories are advantageous over purely simulational methods for several reasons: (i) they describe the processes occurring in particulate mixtures in terms of differentiable quantities, thus allowing the computation of the solution to the problem by methods of mathematical analysis, e.g. finite difference schemes, finite element methods, finite volume, etc.; (ii) they overcome the need to specify exact microscopic configurations—the microscopic effects are captured in terms of macroscopic coefficients or closure relations, e.g. [35,149]; (iii) they can be scale independent of the particle number; and (iv) they do not require an in-depth knowledge of DPMs or experiments. Therefore, in order to have accurately predicting continuum formulations, which are more time-efficient, it is essential that the discrete element simulations emulate—qualitatively and quantitatively—realistic phenomena observed experimentally— thus, bringing us to the following section.

3.1 Comparing experiment and simulation

As has already been noted repeatedly throughout this article, if discrete element simulations and their results are to be of any value to research or industry, they must first be validated through comparison with data pertaining to corresponding 'real-world' systems. Such validation can be achieved, to varying degrees of reliability, by assessing the degree to which one or more of the multitudinous quantities which characterise the state and dynamics of a granular system are observed to resemble one another in simulation and in reality.

In the following sections, we present examples from various studies in which the behaviours of simulated and 'real' granulates are directly compared, focussing on two

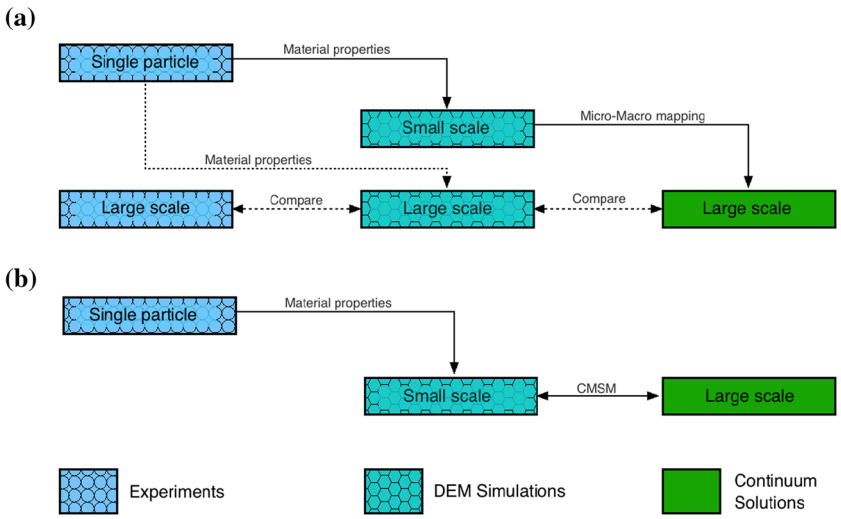

Fig. 2 Comprehensive illustration of the contemporary philosophy adopted by many studies concerning utilisation, calibration and validation of discrete element method [114]. **a** Micro-macro transition **b** Two-way coupling of the continuum and discrete model, also defined as coupled multi-scale mechanics (CMSM)

widely researched experimental setups which are commonly employed in industrial settings— vibrated beds and chute flows. By drawing such comparisons, we aim to build up a picture of the situations in which current simulation models can be 'trusted' to faithfully reproduce real-world systems and, conversely, the cases in which results produced by such models are likely to be unreliable.

3.1.1 Vibrated systems

Vibrated systems are commonly used in industry for various processes such as compaction [150] and the sorting and mixing [151] of powders and granulates, but can also be exploited to provide useful 'model systems' for various natural and biological processes [152,153]. These systems are highly appropriate testing grounds for validating DEM simulations for two main reasons: firstly, compared to 'real-world' systems, and indeed other simplified flow geometries where complex surface and frictional effects are more dominant relative to collisional interactions, vibrated beds are relatively simple. Secondly, experimental setups containing relatively few particles can be made to exhibit most of the important phenomena observed in larger-scale systems [154,155], allowing simulations to be performed quickly and easily. Vibrated systems can also—dependent on the relevant energy input and dissipation control parameters [156,157]—achieve numerous, vastly differing physical states, ranging from jammed, solid-like and glassy configurations exhibiting slow dynamics [158,159] to dilute, highly energetic gases [160,161], thus allowing agreement between experiment and simulation to be verified under various conditions.

We begin by discussing the relatively simple case of dilute, monodisperse systems of spherical particles, where the majority of collisional interactions are binary and contacts between colliding particles are not enduring [162]. In such systems, the specific details of a particle's frictional and elastic properties are comparatively less important [163] and, hence, one may expect simulations to able to recreate the behaviours of experimental systems with comparative ease. Work by Géminard and Laroche [164] looks at what may be considered the 'extremal case' of a dilute granulate—a *single particle* bouncing on a vibrating plate. Their research demonstrates, for this fundamental situation, a strong, quantitative agreement between experimental and simulational results concerning the mean energy possessed by a particle and its scaling with the relevant driving parameters. Specifically, agreement was observed so long as the dimensionless acceleration, Γ, with which the system is driven is greater than or approximately equal to 1.4 (the situation for which, in this system, particle motion is no longer synchronised with base motion). Here, the dimensionless acceleration is defined as $\Gamma = \frac{4\pi^2 f^2 A}{g}$, where f and A are, respectively, the frequency and amplitude of the vibrations by which the system is excited, and g is the acceleration due to gravity—i.e. $\Gamma = 1.4$ corresponds to an applied acceleration 1.4 times greater than gravity. The aforementioned agreement is observed despite the fact that their simulations do not include either sliding or rolling friction coefficients, and assume a coefficient of restitution with no dependence on impact velocity. It is perhaps worth noting that earlier, similar work by Warr et al. [165] showed a significant disagreement between simulation and experiment. Interestingly, however, this is thought by the authors to be due to problems with their *experimental* techniques, as opposed to the limitations of their simulation model—the simulational results acquired were in fact found to agree closely with their theoretical predictions, and indeed the subsequent experimental findings of Géminard and Laroche.

Studies of single particle systems have also shown that more complex behaviours such as period-doubling bifurcations and the transition to chaotic motion may also be successfully reproduced by similarly rudimentary simulations; work by Tufillaro et al. [166], for instance, demonstrates how a simple model assuming frictionless, instantaneous collisions and a constant restitution coefficient can correctly predict the boundaries in frequency-amplitude parameter space which separate the different periodic and chaotic motions exhibited by an experimental system.

We next turn our discussion from single particles to the slightly more involute case of one-dimensional columns comprising multiple individual spherical particles. Once again, simulated systems assuming a frictionless environment and a constant restitution coefficient are shown to be capable of accurately emulating their experimental counterparts. The work of Luding et al. [167], for example, shows that such models can accurately recreate experimental particle distributions, scaling relations and even the presence of *clustering* [168], whereby repeated collisions between imperfectly elastic particles lead to localised increases in the packing density of particles, thus demonstrating that simulations may also faithfully reproduce dynamical processes in which particle collisions are no longer binary, but may involve multiple simultaneous particle contacts.

Simulations concerning dilute granular fluids have also been shown to accurately reproduce experimentally observed phenomena in systems with higher dimensionality. For instance, simulations of two- and three-dimensional systems are capable of reproducing the aforementioned clustering instability [168,169] and the well-known non-Gaussian velocity distributions observed in vibrofluidised granulates [170]—perhaps the two defining features of a granular gas. It is interesting to note that for the case of a *highly constrained, quasi-two-dimensional system*, the inclusion of frictional effects in simulations becomes highly important in producing accurate results [171], while the behaviours of fully three-

dimensional systems can still be accurately represented using frictionless walls and particles [172]. In addition to successfully *reproducing* the known behaviours of granular systems, simulation models have also been used to discover and characterise *new phenomena* unobserved in practical systems. An example of such a discovery is that of low frequency oscillations or LFOs in three-dimensional vibrated systems [173], a phenomenon first discovered using hard-sphere simulations and later confirmed by experiment [174]. A similar model was also used to discover the phenomenon of sudden chain energy transfer events [175,176] in quasi-two-dimensional systems, evidence of which was later observed in experimental, 3D beds [177].

Having established the applicability of discrete element simulations to unary systems in one, two and three dimensions, we now relax the constraint of monodispersity, and explore the degree to which simulation models can successfully characterise the behaviours of dilute systems comprising multiple, distinct particle species. Binary beds, and indeed systems with higher degrees of polydispersity, exhibit various phenomena such as energy non-equipartition [178,179] and segregation [16,180] which are not observed in the monodisperse case, and thus provide additional tests for the validity of discrete element models.

Feitosa and Menon [178] were among the first researchers to directly address the matter of energy non-equipartition, whereby two dissimilar particle species in the *same system* may possess *different kinetic energies*, in violation of the zeroth law of thermodynamics. Specifically, they demonstrated that binary systems of equally sized particles which differ in their masses and elastic properties will exhibit decidedly unequal average energies for the two differing species. The experimental work of Feitosa and Menon was later recreated in simulation by Wang et al. [181] who, unlike in many of the studies previously discussed, implement both a simple friction coefficient for particle interactions as well as a velocity-dependent restitution coefficient. Their setup differs from the experimental case, however, in the introduction of periodic lateral boundaries.

The simulations of Wang et al. were, in the dilute regime, found to reproduce the main features of the experimental system explored by Feitosa and Menon, including the higher concentration of heavy particles observed near the centre of the cell, the well-mixed nature of the system on a local level, the absence of any significant clustering and, most importantly, the divergence in average kinetic energy, $\langle E_K \rangle$ between particle species, with heavier particles possessing greater energy. Moreover, the experimentally observed invariance of the energy ratio between light and heavy particles with base velocity, V, and the consistency of this ratio throughout the bed's central region were also successfully reproduced in simulation.

Although the similarities in the findings of the two studies discussed above strongly hint at the ability of discrete element simulations to successfully reproduce the behaviours of vibrofluidised binary granular mixtures, we nonetheless lack any *direct, quantitative* comparison of simulated and experimental binary systems. Indeed, to the best of the authors' knowledge, there exist few examples of such explicit comparisons in the existing literature.

We aim to address this issue—and other under-investigated systems—by including additional analysis of our own experimental and simulational data acquired from a variety of three-dimensional binary granular beds, assessing the merits and limitations of the application of DEM models to vibrated systems. Our experimental results are acquired using the Positron Emission Particle Tracking technique [34,182], while simulations are performed using the *MercuryDPM* software package [114,183–185].

We look first at the situation investigated by Feitosa and Menon of a binary bed of spheres with equal volumes but differing material properties although we focus on three-dimensional, as opposed to quasi-two-dimensional, systems. The reasoning behind this choice of dimensionality is two-fold: firstly, most granular systems in 'real-world' scenarios are likely to be three-dimensional. Secondly, the dynamical behaviours of three-dimensional systems are more complex than their lower-dimension counterparts—i.e. if the behaviours of these relatively complicated systems can be successfully reproduced in simulation, then we can safely assume them to be capable of describing the simpler one- and two-dimensional cases.

Figure 3 shows the variation with vertical height, z, of the packing density, η, for both components of a variety of different binary systems. Results are shown for experimental datasets alongside corresponding simulations, in which accurate values of the driving vibrational frequency, f and amplitude, A (and hence peak driving velocity, V and dimensionless acceleration $\Gamma = \frac{4\pi^2 f^2 A}{g}$) are implemented, as are known experimental values of particles' elastic coefficients, ε, densities, ρ, diameters, d and hence masses, m.

It is worth noting that ε may perhaps be better interpreted as an informed fitting parameter, as in reality the elasticity of a given collision is dependent on the relative velocity between colliding bodies, in addition to other, more subtle factors relating to particles' material properties and their surrounding environment . The ε values implemented are experimentally determined by measuring the pseudo-instantaneous velocity of a particle immediately before and after a collision with a similar particle. For each particle material used, a number of such collisions spanning a range of relative velocities $0.1 \lesssim v \lesssim 1.0$ ms^{-1} are measured and used to calculate numerous individual values of ε; the elastic coefficient for each particle species is then

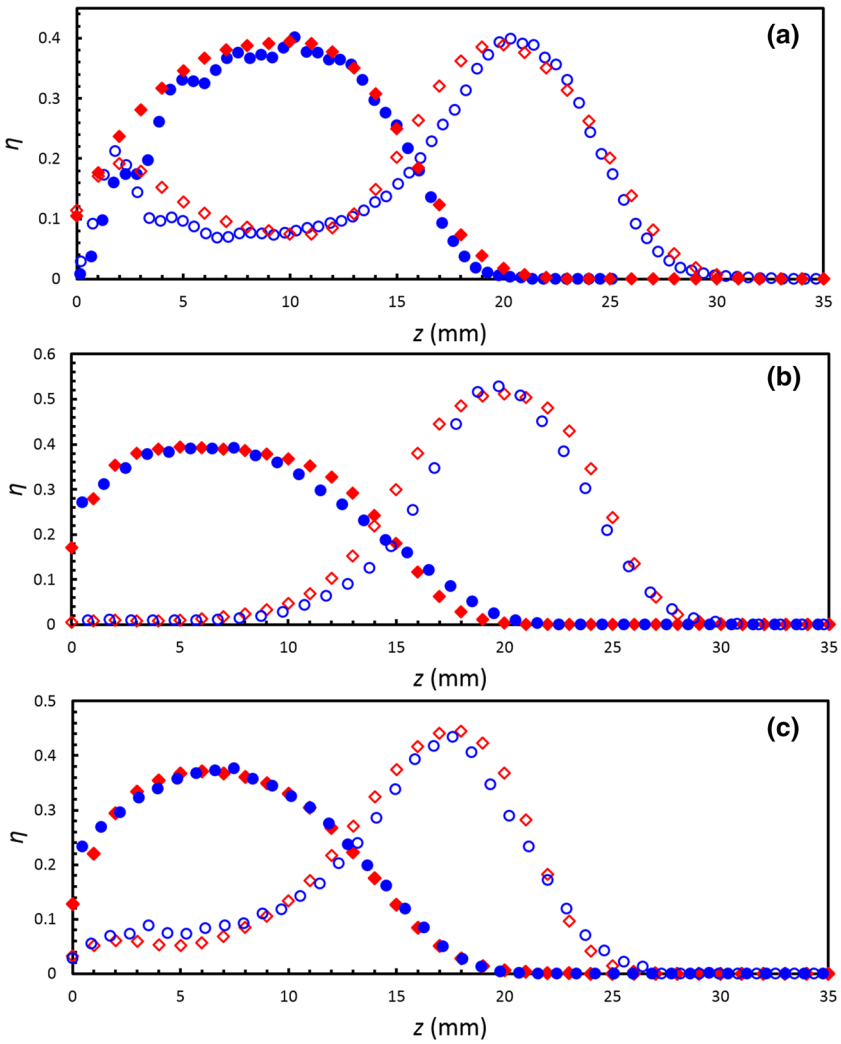

Fig. 3 One-dimensional, vertical packing density distributions for a variety of vibrated, bidisperse-by-material granular beds. Data are shown for **a** a binary mixture of (*light*) glass and (heavy) steel particles driven with a dimensionless acceleration $\Gamma = 6.5$, **b** a binary mixture of (*light*) nylon and (heavy) steel particles driven at $\Gamma = 6.5$ and **c** a binary mixture of (*light*) aluminium and (heavy) steel particles driven with an acceleration $\Gamma = 8$. In all cases, the bed depth, N_L, is equal to four particle layers. Data are shown for experimental results acquired using positron emission particle tracking (*blue circles*) as well as MercuryDPM simulations (*red diamonds*) with, in each instance, *open symbols* representing the particle distribution for the lighter component of the bed, and solid symbols representing heavier particles

taken as the mean of all calculated values for the relevant species.

In fact, the only important system parameters whose experimental values are *not* implemented based on experimental values are the interparticle and particle-wall frictional coefficients, μ and μ_w, respectively, which are assigned a constant value of 0.1. Interestingly, for the strongly fluidised beds explored here, a variation in μ shows little effect on the density profiles produced, while a variation in ε exerts a significant influence, implying that collisional, as opposed to frictional, interactions are dominant in such systems. As is immediately apparent from Fig. 3, a strong agreement between experiment and simulation is observed for all parameter combinations explored, strongly supporting the idea that discrete element simulations are suitable for the numerical reconstruction of relatively well-fluidised, binary granulates.

Not only are the observed profiles qualitatively similar for experiment and simulation, but experimentally acquired values of the systems' time-averaged centre of mass positions (and therefore mean potential energies) agree to well within 10 % with results obtained from simulation. The segregation intensity, I_s—a measure to the degree of species separation exhibited by a system [186]—is also found to agree to within 10 % between experiment and simulation for the systems shown. In other words, we see that our simulations produce strong *quantitative agreement* with experiment, in addition to the qualitative agreement noted in our comparison of the works of Feitosa and Menon and Wang et al.

In fact, the agreement demonstrated in the small selection of images shown in Fig. 3 is observed to persist across considerable ranges of parameter space. Further evidence of the ability of DEM simulations to reproduce the behaviours of experimental systems for a wide variety of system parameters and combinations thereof may be seen in our Figs. 4, 5 and 6. Figure 4 demonstrates the accuracy with which simulations may predict a monodisperse system's particle distribution and, hence, centre of mass position for numerous different combinations of the driving parameters f and A as well as for differing particle numbers, N, and hence bed depths or 'layer

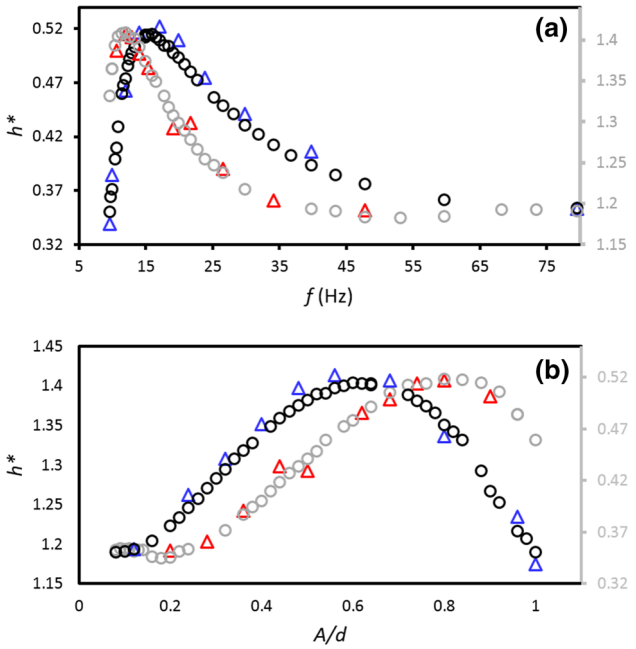

Fig. 4 Fractional increase in the vertical centre of mass position of a granular bed from its resting (unexcited) value as a function of driving frequency, f, and dimensionless amplitude, A/d (with d the particle diameter), for a fixed vibrational energy input, $S \propto V^2$. The fractional increase in centre of mass height is defined as $h^* = \frac{h-h_0}{h_0}$ where h_0 is the bed's centre of mass height for zero driving, and h is its time-averaged, steady state value for a continuously excited system. Data are shown for both experiment (*triangles*) and simulation (*circles*) and for two different bed depths, specifically $N_L = 6$ (*black circles* and *blue triangles*) and $N_L = 3$ (*grey circles* and *red triangles*)

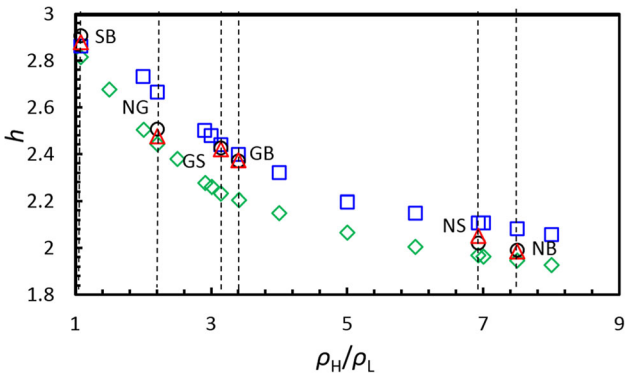

Fig. 5 Variation of the non-dimensionalised vertical mass centre $h = \frac{Z_{cm}}{d}$ with the ratio of particle densities, $\frac{\rho_H}{\rho_L}$, for a series of binary systems of depth $N_L = 5.4$ driven with dimensionless acceleration $\Gamma = 3.5$. Here, $\frac{\rho_H}{\rho_L}$ gives the relative density—and, since all particles used are of equal size, mass—of the heavier (H) particle species to the lighter (L) species for the binary granular mixture corresponding to each data point. Data are shown for experimental (*black circles*) and simulated systems (*red triangles*, *blue squares* and *green diamonds*). The simulations corresponding to the triangular data points represent the 'real' combinations of materials used in experiment, with known values of inelasticity, ε, and density, $\rho_{H,L}$ implemented. Data are shown for binary beds of steel and brass (SB), nylon and glass (NG), glass and steel (GS), glass and brass (GB), nylon and steel (NS) and nylon and brass (NB). Square and diamod-shaped data points, meanwhile, correspond to the case in which only the density ratio between particles, $\frac{\rho_H}{\rho_L}$, is considered, with the particle elasticities held equal at values of $\varepsilon_H = \varepsilon_L = 0.83$ and $\varepsilon_H = \varepsilon_L = 0.41$, respectively. The strong agreement between experiment and simulation for the cases in which experimental ε values are utilised, compared to the considerable divergence observed for cases in which particle elasticities (and the ratios thereof) are held constant, clearly demonstrates the importance of ε to the accurate reproduction of real-world systems using DEM models. Figure taken from our reference [187]

numbers', N_L. The layer number, or 'bed depth', N_L is simply defined as the number of resting layers within a system (i.e. the number of layers formed when the system is exposed to zero excitation) normalised by the particle diameter, d. In Fig. 5 we see that the agreement between simulationally and experimentally obtained values of the vertical mass centre persists also for the more complex case of binary systems, successfully accounting for variations in particle density and elasticity and, indeed, the combinations thereof for differing binary mixtures. In particular, this figure provides a stark illustration of the importance of particle inelasticity to the behaviour of granular systems, and hence the necessity of the correct implementation of this property in computational models.

In Fig. 6, meanwhile, we compare simulated and experimental segregation intensities, I_s, achieved by systems in their steady states. Data are once again shown for various combinations of particle material. This image provides a fascinating insight into the importance of implementing accurate values for particles' restitution coefficients, as simulated and experimental results are observed to diverge sharply when differences in ε are not accounted for, even when all other system parameters are accurately implemented.

We have, thus far, demonstrated that DEM simulations are highly capable of accurately reproducing, both qualitatively and quantitatively, the physical properties and dynamical behaviours of relatively *dilute, well-fluidised* monodisperse and binary systems in one, two and three dimensions. However, as we tend towards the high-density limit in which the condition of fluidisation is no longer fully upheld and systems experience an increased prevalence of enduring contacts and a greater influence due to frictional interactions, the simplified force models adopted by DEM simulations face a more stringent test.

Returning to the case of a simple, one-dimensional column—where frictional effects between particles are limited due to the restricted angle of impact between particles—we once more find that simulations can quantitatively reproduce bed behaviours; Fig. 7, for instance, shows that—as with the dilute case—the gravitational potential energy of a system can be accurately predicted for a range of driving parameters and system sizes. Simulations are also found to accurately predict quantities such as the frequency of the periodic motion achieved by dense systems under specific

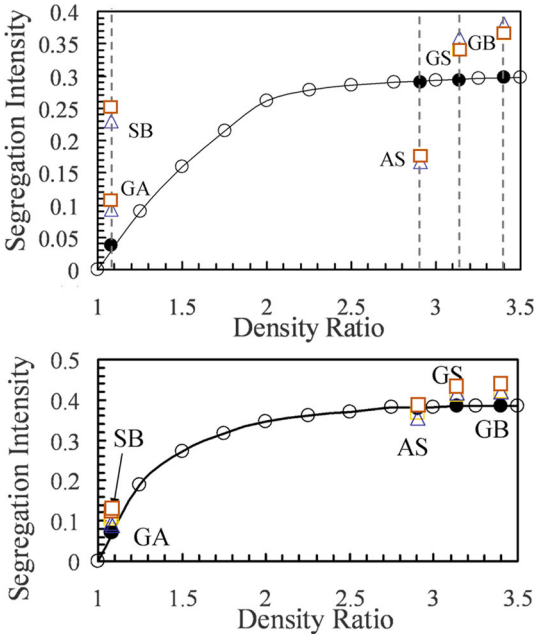

Fig. 6 Variation of segregation intensity, I_s, with the density ratio, $\frac{\rho_H}{\rho_L}$, of particles in a variety of binary granular systems. For all cases represented in this Figure, a segregation intensity of zero represents a perfectly mixed system, while a value of 0.5 indicates a fully separated bed. Data are shown for beds of depth $N_L = 2.5$ (*top*) and $N_L = 10$ (*bottom*), both systems driven with a constant dimensionless acceleration $\Gamma = 17$. In both panels, experimental data are represented by *triangles*, while *squares* represent simulations in which experimental density and inelasticity values are implemented and *circles* represent the case in which segregation is driven purely by density differences ($\varepsilon_H = \varepsilon_L = 0.91$). Filled circles correspond to experimental density ratios, once more demonstrating the considerable discrepancy between simulation and experiment when inelasticity effects are not considered. As with Fig. 5, experimental particle combinations (and the simulations in which the relevant experimental parameters are implemented) are specifically labelled, with data here been shown for combinations of steel and brass (SB), glass and aluminium (GA), aluminium and steel (AS), glass and steel (GS) and glass and brass (GB). Figure taken from our reference [188]

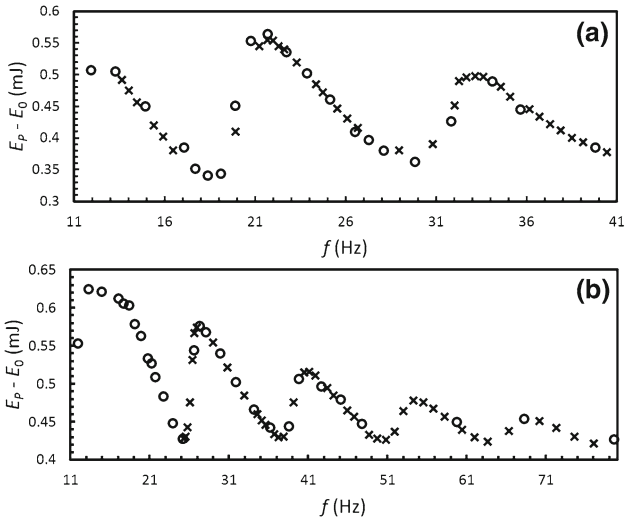

Fig. 7 Time-averaged gravitational energy, E_P, for a column of particles exposed to continuous vibrational energy input as a function of the oscillatory frequency, f, of the moving wall providing energy to the system. As with Fig. 4, data are shown for a fixed energy input ($S = \frac{4\pi^2 f^2 A^2}{gd} = 1.83$) achieved through a variety of f-A combinations. Data are shown for one-dimensional columns comprising 15 particles (*top*) and 20 particles (*bottom*), presenting in each case both experimental (*circles*) and simulated (*crosses*) datasets. In each panel shown, the resting gravitational potential energy, E_0, possessed by the bed at zero energy input is subtracted from E_P in order to isolate the potential energy gained by the system through the applied vibrational excitation. Figure taken from our reference [189]

driving conditions. Other studies have shown that, in addition to the global properties mentioned above, simulations may also closely reproduce the internal dynamics of a columnar system on the 'microscopic' level—work by Rosato et al., for instance, has recently demonstrated that the experimentally measured [190] speed of a compression wave through an excited granular column may be correctly determined in simulation [191]; the impressive agreement observed between experiment and simulation provides a pleasing example of the ability of non-Herzian contact models to accurately reproduce physical processes even in relatively dense systems.

Studies of two-dimensional systems also show a continued strong agreement between simulations and experiment in the high-density case. Work by Yang and Hsiau, for instance, shows an impressive quantitative agreement between experimental and simulated velocity distributions [192] as well as close correspondence regarding the diffusive behaviours and granular temperatures [193] of dense, two-dimensional beds. Venturing further towards the high-density limit, where particle motion becomes less fluid-like and granular beds begin exhibiting crystallisation [194] and glassy properties [195], the strong similarities between experiment and simulation are still found to persist. Studies have found, for instance, that the *solidus point*—the filling fraction for which a granular bed 'freezes'—observed for a two-dimensional experimental system agrees quantitatively well with that pertaining to a simulated system of discs [196,197]. It is rather remarkable that such a strong, quantitative agreement is observed here in spite of several considerable differences between the experimental and simulated systems investigated, in particular the differences in particle dimensionality, with three-dimensional spheres used in experiment and two-dimensional discs modelled in simulation, and the fact that while experimental granulates are inherently non-equilibrium systems, the simulations to which they are compared correspond to an equilibrium state. Simulation are also found to successfully and accurately capture the *structural configuration* of dense, two-dimensional systems, as demonstrated by a strong agreement between experimentally acquired and simulated radial distribution functions and shape factors [197–199]. In fact, the only deviations

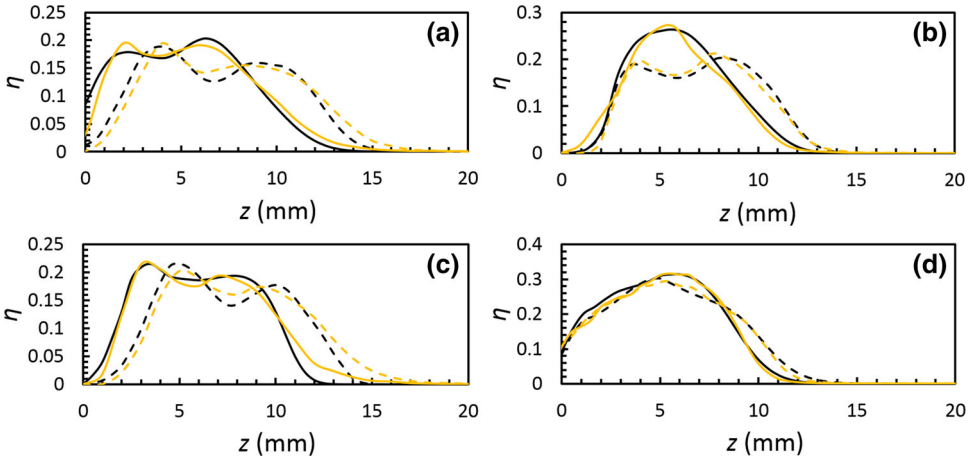

Fig. 8 Packing density profiles for a variety of binary granular systems comprising particle species equal in volume and density (and hence mass) but differing in geometry. Data are shown for systems of **a** spheres and cuboids driven at a frequency $f = 40$ Hz and an amplitude $A = 1.67$ mm, **b** cuboids and disc-like particles driven with the same f and A as the previous system, **c** spheres and cuboids driven with $f = 100$ Hz and $A = 0.67$ mm and **d** spheres and cuboids driven with $f = 80$ Hz and $A = 0.42$ mm. In all cases, a dimensionless bed height $N_L = 2.5$ is used. For all images shown, particles possessing a higher radius of gyration, r_g, (i.e. larger 'effective size' [204,205]) are represented by dashed lines, while solid lines correspond to lower-r_g species. Figure taken from our reference [206]

between the experimental and simulational results of the cited articles are thought to arise simply due to the imperfectly two-dimensional nature of the experimental system studied, leading to a finite number of out-of-plane collisions between particles and hence overlap in the resulting projections used to determine particle distributions. In other words, for a perfectly two-dimensional experimental setup, one may well expect a near-perfect agreement across the full range of system parameters.

For the case of fully three-dimensional granular beds, it becomes increasingly difficult to conduct direct, quantitative comparisons of the behaviours of simulated and experimental particulate systems. Interestingly, the difficulty in comparison arises largely from the limitations of the currently available *experimental techniques* as opposed to the limitations of contemporary computational methods. For instance, at high packing densities, the high collision rate between particles makes it highly difficult to resolve particles' instantaneous velocities due to limited data acquisition rates of experimental equipment [200,201], while the opacity of a densely packed system will clearly render the real-time imaging of a three-dimensional system's interior considerably more complicated. Nonetheless, parameters such as mean squared displacement (MSD)— which reduce the noise associated with direct measurement of particle velocities—have been shown to produce a pleasing qualitative agreement between simulation and experiment in both two- [201] and three-dimensional [202] systems. Other behaviours, such as the time-dependent compaction of a granular bed and the variation of particle mobility with packing density, are also found to be qualitatively reproduced by simulations [203]. Although the existing literature— and indeed our own findings—show that DEM simulations are capable of emulating their experimental counterparts on a qualitative level, there exists, at present, little conclusive evidence to either support or disprove the ability of such simulations to provide a full, quantitatively accurate reproduction of dense, three-dimensional, vibrofluidised systems.

We have thus far assessed the viability of discrete element simulation models across a broad spectrum of system parameters and dimensionalities. However, all of the research discussed up to this point pertains to granulates composed entirely of *perfectly spherical particles*. As we have previously mentioned, 'real' particle flows observed in industry and nature will seldom be composed of exclusively spherical constituents. However, as we have repeatedly observed from the studies discussed above, a simulation does not necessarily have to precisely match its experimental counterpart in terms of particle geometry and material properties in order to elicit an accurate, quantitative reproduction of the system's dynamical behaviours and structural properties. This fact is exemplified in our reference [206] where it is shown that the particle distributions and segregative behaviours of binary systems comprising particles differing both in *density and geometry* may be accurately and quantitatively reproduced using simulations of *solely spherical particles*. An example of the close agreement observed is depicted in Fig. 8. The simulated density profiles shown in Fig. 8 account for changes in particle geometry through an appropriate alteration of the diameter of the spherical particles modelled, based on the radii of gyration [207–209] of the non-spherical shapes used in experiment, and an alteration of the parti-

cles' restitutive coefficients, taking into consideration the additional translational kinetic energy lost to the rotational modes [210]. For the case of *gaseous systems*, where contacts between particles are near-instantaneous, agreement between simulation and experiment is strong for a variety of particle geometries and materials, across a range of driving parameters. However, for increasingly dense beds where systems become sensitive to the more specific aspects of interactions between particles as well as the differences in packing density achievable by shapes of differing geometries [211,212] this simple model is, rather unsurprisingly, found to fail.

In recent times, a number of simulation codes have been developed which are capable of directly modelling particles of various diverse geometries. Although inherently less computationally efficient than simulations involving only spherical particles, these algorithms allow a deeper investigation of the influence of particle shape on the behaviours of vibrated granulates across an increased range of parameter space.

Perhaps the simplest non-spherical geometries to numerically model are spherocylinders and ellipsoids, due at least in part to the relatively simple contact detection algorithms required [213,214]. Prior studies have shown that DEM simulations using these particular particle shapes can provide a close, quantitative agreement with experiment, with work by Pournin et al., for instance, successfully reproducing the self-assembly of a bed of spherocylindrical particles experimentally observed by Villarruel et al. [215]. Even for the relatively complex case of a densely packed, fully three-dimensional system, a comparison of the two studies shows quantitative agreement in terms of the initial and final packing densities achieved and even the timescales corresponding to the ordering processes within the systems explored. Beyond the constraints of ellipsoidal/spherocylindrical geometries, there exists an apparent lack of DEM-based research focussing on vibrated systems with more complex non-spherical constituents, despite the existence of numerous such studies pertaining to sheared beds [216,217] and gravity flows [218,219], for instance. Recently, however, the *multi-sphere method* [220], which has proved highly effective in the modelling of other system geometries [221–223], has begun to be applied to vibrated and vibrofluidised beds. Using the multi-sphere approach, each non-spherical particle within a system is composed of a number of smaller objects, creating 'composite particles', the modelling of which is often more computationally efficient than for complex shapes represented using single particle models [224,225]. Work by Chung et al. [226], for example, demonstrates, for the case of simple paired particles, an excellent, quantitative agreement between experiment and simulation, providing strong support for the validity and applicability of the multi-sphere model in vibrated beds. Pei et al. [227], meanwhile, implement more complex elongated particles comprising spheres of differing sizes. They study the effect of geometry on the transfer of electrostatic charge between particles, finding their results to agree qualitatively with experimental expectations.

Qualitative predictions arising from numerical studies using the Monte Carlo method [207] to simulate the segregative behaviours of particles possessing still more complex geometries also agree well with experimental observations [206]. Although these simulation methods can at best be described as semi-quantitative, the observed correspondence between experiment and simulation nonetheless shows promise.

In summary, we have demonstrated that numerical simulations of vibrated and vibrofluidised granular beds can provide quantitatively accurate models of the behaviours of these systems over a wide range of parameter space. The models used are capable of recreating numerous complex behaviours exhibited by particulate systems spanning one, two or three spatial dimensions, existing in solid-like, liquid-like or gaseous states and comprising particles possessing various diverse material properties. While there remain certain cases where the applicability of particle simulations is yet to be fully verified, with the continuing improvements in processing power, in addition to the further refinement and development of the computational methods and contact models associated with DEM simulations, it is likely that these remaining issues will be resolved in the not-too-distant future.

3.1.2 Flows over inclined channels (chute flows)

Similar to vibrated systems, inclined channels (chutes) are also commonly employed in various industrial processes, for example in the mining, pharmaceutical and food-processing industries, which handle particulate media [2]. Besides their numerous industrial applications, a range of geophysical events (including avalanches, landslides, debris flows... [228–230]) can also be emulated utilising this simple flow geometry. Hence, a thorough understanding of the relevant granular dynamics is not only vital for designing efficient handling equipments but also for developing accurate continuum formulations used to predict these hazardous natural events.[5]

Attributable to the inherent nature of granular materials to exhibit a range of diverse behaviours, they are broadly categorised into three regimes: solid, liquid and gaseous (see Figs. 9, 10). Vibrated systems (Sect. 3.1.1) can, under certain circumstances, fall into the category of gases because the particulate media is dilute and the grains interact through binary collisions. However, as stated earlier in Sect. 3.1.1, depend-

[5] These continuum formulations can also be used to model industrial flows.

ing on the amount of energy input and the chosen dissipation parameters, these systems can appear to be solid- or liquid-like as well. In contrast to vibrated systems, granular flows over inclined channels fall in the category of intermediate liquid regimes where the flows are rather rapid and dense—high volume fraction—where the momentum exchange and energy dissipation is due to both collisional (instantaneous) and frictional (enduring) contacts between particles. This section focusses solely on the dense liquid flow regime. Essentially, a granular material is a conglomerate of multiple discrete, solid constituents which are typically dispersed in a fluid. In dense flows, the particles are much denser than the interstitial fluid with low dispersion (closely packed). As a result, the interstitial fluid, e.g. air, is often neglected as it has negligible effect on the bulk flow behaviour. Despite such simplicity, the behaviour of these dense rapidly flowing dry particulate media is yet to be completely understood.

In order to gain an improved understanding, studies have utilised a varied range of experimental setups—plane shear, annular shear cell, vertical chute, rotating drum, heap flow, inclined channel (our current interest)—in which the granular material is subject to simple shear. For the schematics of these setups, see [232]. By employing the available state-of-the-art experimental techniques such as particle imaging velocimetry (PIV) [115], particle tracking velocimetry (PTV) [233], force sensors [234,235], acoustic probes [236], tracked transmitters [237], capacitance probes [238], optical imagery [239], digital imaging [240–242], refractive index methods (RIM) [243], X-ray tomography [244], magnetic resonance imagery [245], studies have not only determined the kinematic properties but also the rheological behaviour of dense granular flows. However, no contemporary experimental technique has the ability to directly determine the local or global stresses generated in such flows. In contrast, discrete element simulations are able to provide all the useful information necessary to fully understand the dynamics of a system—hence this indispensable need for cooperation and agreement between experiments and (discrete element) simulations.

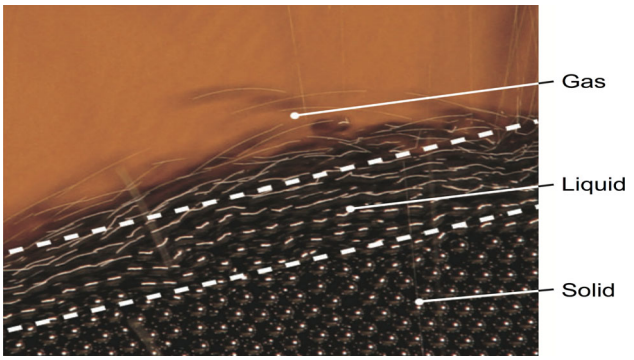

Fig. 9 The above figure, adopted from Forterre & Pouliquen [231], illustrates three flow—solid, liquid and gas—regimes attained by pouring glass beads on a pile

Although simple, understanding these flows has been a daunting task. We begin with a relatively simpler case of monodisperse flows over both smooth and rough inclined channels. Interests in understanding these flows date back to the 1970's where several studies [246–250] focussed on determining the rheological properties (constitutive laws) of mixtures constituting sand or glass beads. Followed by Hwang and Hogg [251] and Brennen et al. [252], where the former focussed on examining the diffusive remixing in these flows while the latter illustrated the possibility of granular jumps or bores. However, due to the lack of intrusive experimental techniques to precisely determine the flow velocity, solid volume fraction and granular temperature, studies approached computer simulations as an alternative approach, see [253,254] and the references therein. Campbell et al. [253,255] were the first to compare their particle simulations of two-dimensional unidirectional flow of inelastic circular cylinders with experiments. They used a hard-sphere DEM approach and observed their results to qualitatively match the findings of Augenstein and Hogg [249] but not of Savage [250] and Ridgway and Rupp [246]. While majority of the studies focussed on understanding the fundamentals [256–262] and developing continuum formulations [145,263,264],

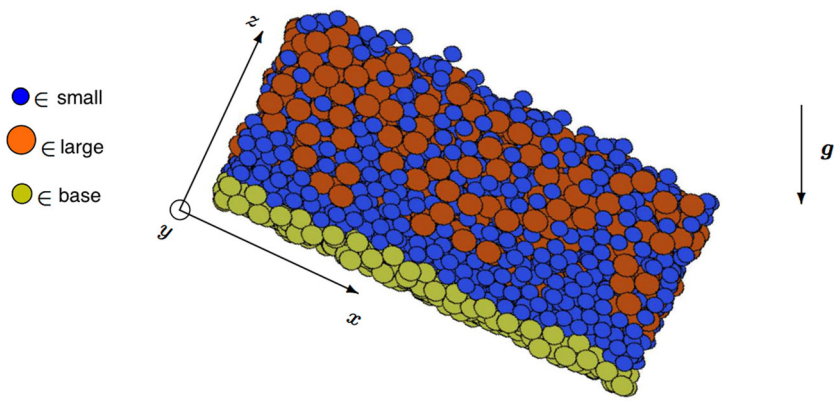

Fig. 10 A snapshot of a periodic *box* containing bidisperse mixtures flowing over rough inclined channels. The *box* is utilised to simulate infinitely long inclined channel flows

it was in the early 1990's where discrete element simulations were employed to analyse two-dimensional [265–267] and three-dimensional [268] flow behaviour of inelastic frictional particles. However, most of these simulations either constituted very few number of particles [265–267] or were not fully steady [265].

In the early 2000s, few of the calibration steps illustrated in Fig. 2a were pursued to investigate flows of glass beads over a rough inclined channel [269]. Using a combination of experiments and discrete element simulations, Hanes and Walton [269] studied the effects of basal and side-wall roughness on the flow structure and its dynamics. In their experiments, steady flows were observed for a range of inclinations. Furthermore, for two inclinations, the particle velocities (both near the side-walls and at the free-surface), the mass flow rate and the flow depth were found to be in relatively good agreement with discrete element simulations. Furthermore, their DEM simulations utilised the contact parameters for glass beads which were determined using single particle experimental measurements carried out by Lorenz et al. [270]. Similarly, several other studies [35,149,271,272] have used DEMs to simulate both steady and unsteady flows of cohesionless particles (glass beads) and found them to be in good agreement with experimental observations. Silbert et al. [271,273] investigated the rheology of fully three-dimensional, steady, dense flows of cohesionless frictional spheres over rough inclined planes. The channels are made rough by sticking particles on the channel surface, over which the material flows. Among the areas studied were the effects of parameters such as interparticle friction coefficient, inelasticity, flow heights and channel inclinations. Steady flows were found to exist over a wide range of inclination angles and heights confirming the experimental observations of Pouliquen [148]. For different flow heights (thick flows), Silbert et al. [271] found the flow properties such as velocity and strain-rate to be sensitive to the interparticle friction coefficient. Additionally, for thick enough flows the velocity profiles and rheology were shown to adhere to Bagnold scaling. However, as one gradually reduces the flow height, Silbert et al. [273] observed transitions from Bagnold rheology to linear velocity profiles which are consistent with the experimental observations of Lemieux and Durian [274] (avalanches), Ancey [275] (linear velocity profiles) and Pouliquen [148] (Bagnold scaling). Furthermore, Silbert et al. [273] observed that both the thin and thick flows obey a simple scaling law consistent with the experiments of Pouliquen [148]. In addition to the range of parameters, stated previously, considered to understand their effects on these flows, Weinhart et al. [35] and Thornton et al. [149] investigated the effects of varying basal properties. By changing the basal particle diameter or interparticle friction between the flowing particles and fixed base particles, [35,149] studied the effects on the effective macroscopic friction coefficient. For varying basal particle diameter, Weinhart et al. [35] found their simulation results to be in good agreement with the empirical law determined by the experiments of Pouliquen and Forterre [148,276]. Not only did Weinhart et al. [35] obtain a DEM validated empirical law for the effective macroscopic friction coefficient, but they also determined other closure relations such as the ratio of the stress in the downslope and normal direction (flow depth), K, mean flow density, $\bar{\rho}$ and the shape of the velocity profile, α,—essential for solving the continuum shallow-layer granular continuum model [145,147]. Similarly, for varying basal contact friction coefficient, Thornton et al. [149] presented a modified empirical law [276] which could be used in continuum models to simulate flows over varying base types, i.e. rough or smooth. In addition, by choosing the right interparticle collision model and contact parameters, recent experimental studies have further validated discrete element models of monodisperse glass spheres over non-rotating [277] and rotating smooth inclined channels [116,278], thereby illustrating the current ability and future potential of discrete element simulations to emulate and understand monodisperse flows over both smooth and rough inclined channels. For more examples and a detailed review concerning other applications of discrete element simulations, see [74,232].

As stated earlier, real-world flows comprise particles of varied sizes, densities, shapes and many other characteristic features. Attributable to these varied features, particles in dense rapid flows (also in vibrated systems) tend to arrange themselves in distinct patterns [10,281–284]. This phenomenon is known as particle segregation. Despite these varied particle attributes, differences in size are considered to be the most important, see [283,284] and references therein. Similar to the interests shown in understanding monodisperse flows, several experimental studies have also attempted to address the issue of size-based particle segregation in rapid dense flows over inclined channels [263,277,285–291]. It was in the late 1990's when a two-dimensional discrete element simulation of inelastic discs was carried out to quantitatively describe the segregation phenomenon. However, no quantitative agreement was achieved between the experiments of Savage and Lun [263] because of the different mixture compositions considered. While most of the studies focussed on developing accurately predicting continuum segregation models using DEMs, Thornton et al. [184] illustrated the need of a frictional tangential force collision model for producing steady flows with strong segregation as seen in experiments. Interestingly, similar results were also produced simply by adding tangential dissipation to the contact model. Although they were able to observe realistic flow behaviours, further investigation is necessary to investigate the effects of chosen contact models on segregation. Recently, by systematic fine tuning (parameter calibration) of the contact model, Bhat-

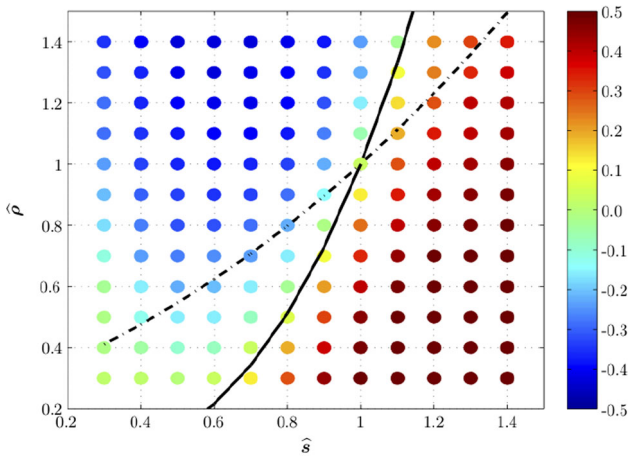

Fig. 11 The above phase-plot is constructed using several fully three-dimensional periodic-box DEM simulations of bidisperse mixtures, i.e. mixture comprising of two types of particles. Using a simple force model, homogeneously mixed bidisperse mixture, for a range of size and density ratios, is allowed to evolve till steady state is reached. Given $\widehat{s} = s^2/s^1$ and $\widehat{\rho} = \rho^2/\rho^1$ is defined as the size and density ratio, the above illustration plots normalised relative vertical centre of mass, $\widehat{D}_{com} = (z^2_{com} - z^b_{com})/z^b_{com}$. z^2_{com} is the vertical centre of mass of type-2 particle, whereas z^b_{com} is the bulk's vertical centre of mass. As an example case, for a purely size-based mixture $(\widehat{s}, \widehat{\rho}) = (1.4, 1.0)$, we have $\widehat{D}_{com} = 0.5$. Implying that the large particles (type-2) rise towards the free-surface, whereas the small particles (type-1) settle near the base of the flow. Similarly, we plot $\widehat{D}_{com}$ for different $\widehat{s}$ and $\widehat{\rho}$. Additionally, the solid line denotes the line of weak segregation predicted from the continuum theory model of Tunuguntla et al. [279], whereas the dotted-dashed line is the weak segregation line predicted analytically by Jenkins and Yoon [280] using kinetic theory. For more details see Tunuguntla et al. [279]

tacharya and McCarthy [277] showed quantitative agreement with the experiments. While purely size-based segregation has been a topic of interest for several years, Tunuguntla et al. [279] investigated both size *and density* effects on segregation, see Fig. 11. Although no direct quantitative comparison were made with experiments, qualitative agreements were found with the experiments of Felix and Thomas [286]. These results imply that, with proper calibration of DEMs, one should be able to effectively emulate the experimentally observed particle phenomena on a quantitative level.

Although studies have shown particle shape to have significant effects on particle dynamics, there exist very few studies concerning the experimental validation of DEMs of non-spherical particles flowing over inclined channels. Nevertheless, by proper calibration, Vu et al. [292] illustrated the ability of DEMs to simulate flowing ellipsoids in an attempt to simulate the dynamics of flowing soybeans, their results being further validated by experimental findings. However, additional validation of particle simulations is required to comfortably apply them to analyse the complex flows of non-spherical particles.

4 Summary and conclusions

Through analysis of the extensive literature relating to the computational modelling of granular and particulate flows, we have provided an overview of the extent to which current discrete element simulations may successfully emulate the behaviours of dynamic experimental systems, focussing specifically on vibrofluidised beds and chute flows—two systems with direct relevance to numerous natural and industrial processes.

We have carefully examined the specific circumstances under which computer models may—if correctly implemented—be expected to accurately recreate experimental systems for two commonly explored types of granular flow. We show that simulations of *vibrated* systems produced using the discrete element method are capable of quantitatively predicting the behaviours of granulates in one-, two- and three-dimensional systems, for the case of monodisperse beds and bidisperse mixtures, and for systems in dilute gaseous states, liquid-like states and densely packed solid-like states. Discrete element models of *chute flows*, meanwhile, are found to show strong quantitative agreement with experiment for monodisperse flows across flat, bumpy, frictional and smooth surfaces for all dimensionalities. The segregative behaviours of binary systems which are bidisperse-by-size have also shown to be correctly simulated using the discrete element method, although agreement between simulated and experimental systems comprising particles of differing densities remains to be directly tested.

Perhaps the most pressing open question for both vibrated granular systems and chute flows is whether the effects of particle *shape* can be adequately captured by simulation models. At present, although quantitative agreement has been observed for very simple systems, and qualitative trends reproduced for more complex cases, there exists insufficient direct evidence to concretely confirm or deny the suitability of current models to the task of modelling non-spherical systems. Considering that the majority of particles involved in real industrial and natural processes possess non-spherical geometries, this is most certainly an issue worthy of direct, systematic research in the future.

In summary, the collected works discussed here demonstrate the ability of discrete element simulations to successfully emulate experimentally observed phenomena exhibited by dry granular media in both vibrated beds and liquid regimes (chute flows). In doing so, we show that such simulation models provide a potentially powerful tool with which we may better understand and predict the behaviours of granulates in these commonly used flow geometries. The successful application of DEM models to these canonical systems suggests that they may indeed prove equally valuable in other granular systems.

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