

# Heterarchical granular dynamics: state of the art

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**Abstract.** Heterarchical Granular Dynamics (HGD) represents a new approach to modelling the complex behaviour of granular materials across multiple scales. By modelling granular materials stochastically, HGD has enabled the simulation of granular phenomena ranging from simple systems to highly dynamic processes such as comminution in rotary mills. This summary reviews the foundational assumptions and key mechanisms underpinning HGD. Unlike the discrete element method, HGD efficiently scales to industrially relevant numbers of particles, and unlike traditional continuum methods, it retains microstructural information. HGD continues to evolve as a versatile framework for understanding granular dynamics in both natural and industrial contexts.

## 1 Introduction

Traditional computational approaches for modelling granular materials have relied primarily on two families of tools: discrete simulations, such as the discrete element method (DEM) [1], where individual particles and their interactions are modelled, and continuum mechanics-based models such as the finite element method (FEM), smoothed particle hydrodynamics (SPH) and the material point method (MPM) [e.g., 2, 3].

For systems with small numbers of particles ( $\lesssim 10^7$ ), DEM can be used to describe the motion of every individual particle within the assembly. Unfortunately, for many industrial and natural systems,  $10^7$  is often significantly smaller than the number of particles present (e.g., there are  $10^6$  fine sand particles per  $\text{cm}^3$  at a beach) and computational limitations significantly hinder scalability. Conversely, continuum models offer computational efficiency but often fail to account for the complex microstructural dynamics that govern granular behaviour, particularly in highly polydisperse or evolving systems. These challenges have catalysed the development of a novel modelling paradigm: Heterarchical Granular Dynamics (HGD) [4].

HGD introduces an alternative framework that integrates stochastic dynamics and multi-scale modelling to bridge the gap between micro- and macro-scale behaviours. Unlike hierarchical models that maintain a strict separation between scales (e.g., FEMxDEM couplings [5, 6]), heterarchical models allow for dynamic information exchange across scales through internal microstructural coordinates orthogonal to traditional spatial and temporal dimensions. This allows for the simultaneous consideration of processes occurring at different scales, such as particle breakage, segregation, mixing, and their feedback on the bulk behaviour.

The conceptual underpinning of HGD lies in its departure from traditional hierarchical modelling ap-

proaches. Hierarchical models typically enforce a uni- or bi-directional flow of information between finer and coarser scales. This connectivity between scales limits the ability to exchange information between locations *at the same scale*. However, the breakdown of clear scale separation is a hallmark of granular media.

In contrast, HGD employs a heterarchical structure (see Figure 1), characterized by dense connectivity between scales and at the same scale. This is achieved through the introduction of internal microstructural coordinates that exist orthogonally to the conventional spatial and temporal dimensions.

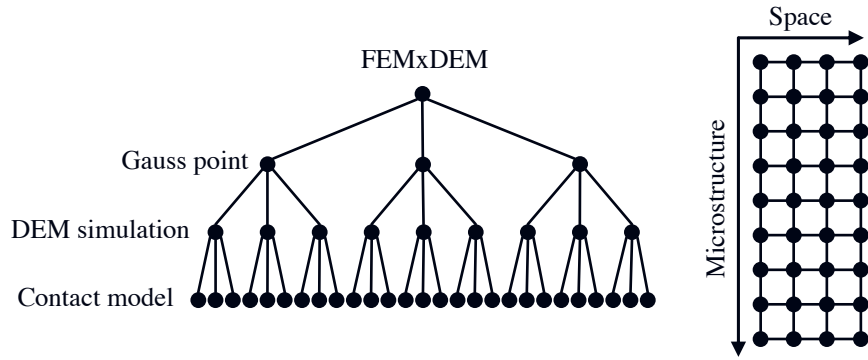
The heterarchical approach relies on defining a state space where traditional spatio-temporal coordinates ( $x, y, z, t$ ) are augmented with a microstructural coordinate  $m$ , representing properties such as the grain size distribution, contact network topology, and local voids.

This work aims to provide a comprehensive overview of the state-of-the-art in HGD, highlighting key mechanisms that have been modelled such as comminution, segregation, mixing, and void migration. We explore the mathematical foundations of HGD and its applications in both natural and engineered systems.

## 2 Model formulation

To date, HGD models have been formulated on both regular cartesian lattices [4, 7–9] and on unstructured meshes [10, 11]. Within this paradigm, two sets of models have been produced. The first, chronologically, have ignored the void spaces, and have dealt solely with the motion of the solid phase. These models have all required *a priori* knowledge of the motion of the material. More recently, in [4], a new formulation was derived which includes void spaces in the model, and subsequently the motion of the material can be predicted dynamically. Here, we outline only this most recent formulation, and put the

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**Figure 1.** Conceptual comparison of hierarchical (left) and heterarchical (right) modelling frameworks.

mathematical formulation proposed in [9] into this framework.

We discretise an  $N$ -dimensional physical space into an  $(N + 1)$ -dimensional cartesian grid, including an additional microstructural coordinate. For two spatial dimensions  $(x, y)$  and a microstructural coordinate  $m$ , at any point in this discrete space  $(x, y, m)$ , we have cells of equal volume. We require that each cell contains either (1) particles of a single size, or (2) a void. We represent the size (diameter) of the particles in that cell as  $s_{i,j,k}$ , where  $i, j$  and  $k$  are the indices in the respective dimensions. If the cell contains void space, we set  $s_{i,j,k} = 0$ . In this way we can, for example, calculate the porosity  $n$  at any point in physical space  $(i, j)$  by taking the average number of voids, as

$$n_{i,j} = \frac{1}{M} \sum_{\substack{k=1 \\ \forall s_{i,j,k}=0}}^M 1, \quad (1)$$

with  $M$  the number of cells in the  $m$  direction. The solid fraction can then be defined as  $\nu = 1 - n$ . Similarly, other representative measures such as the grain size distribution can be calculated by taking averages over the microstructural coordinate.

Typical practical guidelines for discretisation parameters involve choosing cell sizes sufficiently small to capture the relevant particle-scale interactions, yet large enough to remain computationally efficient. Generally, selecting 20 – 200 cells along the microstructural coordinate ensures reasonable representativeness and accuracy. With increasing number of cells, the model converges towards an equivalent continuum description (see Section 3.2.4), and the criterion of 20-200 cells represents an approximate range at which this begins.

## 2.1 Representativeness

We define a “representative” scale, in the sense of a representative volume element, to be an average over the microstructural direction. In this way the porosity, defined above, is taken to be representative, but the local configuration of sizes or voids is not. Similarly, we can define the discrete grain size distribution  $\phi(s_a)$  as by counting the number of cells with sizes in a size range  $s_a \pm \Delta s$ , at a location  $(i, j)$  as

$$\phi_{i,j}(s_a) = \frac{1}{\nu M \Delta s} \sum_{k=1}^M \mathcal{H} \left( \frac{\Delta s}{2} - |s_{i,j,k} - s_a| \right), \quad (2)$$

where  $\mathcal{H}$  is the Heaviside step function. The arithmetic average size across the microstructural coordinate can then be defined as

$$\bar{s} = \frac{1}{\nu M} \sum_{\substack{k=1 \\ \forall s_k \neq 0}}^M s_k. \quad (3)$$

## 3 Physical mechanisms

HGD models the complex interplay of various mechanisms that govern the behaviour of granular materials. To date, these mechanisms have been limited to particle breakage, segregation, mixing, and void migration.

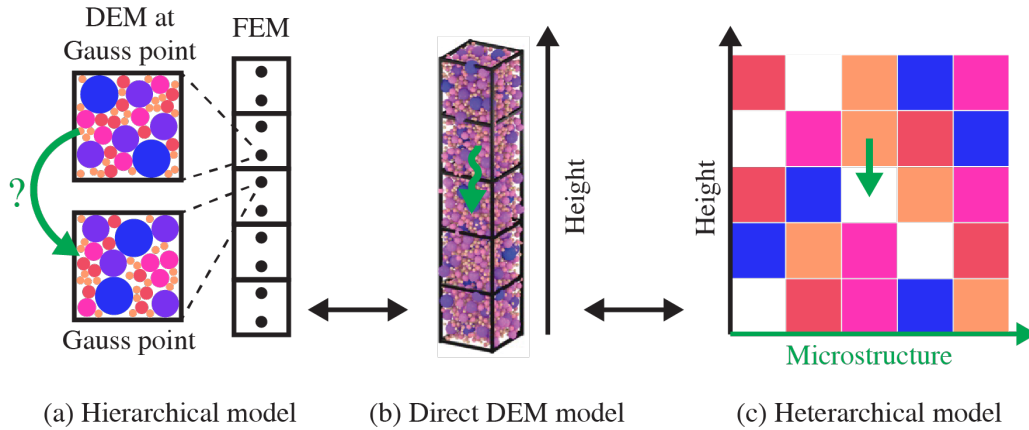
### 3.1 Closed systems

We begin with mechanisms that can be considered to affect “closed” systems, where no mass enters or leaves the representative volume, and changes only occur within it.

#### 3.1.1 Particle breakage

Particle breakage causes a reduction of particle size due to mechanical stress exceeding particle strength. This is a process that is critical in both natural systems (*e.g.*, fault gouges, landslides) and industrial applications (*e.g.*, rotary mills, cement production). In HGD, particle breakage is modelled as a stochastic process influenced by the local stress environment, material properties, and microstructural configuration. The primary driving forces modelled to date are static [9] and dynamic [10] stresses that exceed the material’s strength, leading to particle breakage.

The local configuration of each particle is important to determine its likelihood of breaking under a particular static loading condition [12]. Particles that have many contact points are on average more likely to experience isotropic compression, and are typically shielded from experiencing significant internal tensile stresses, and hence



**Figure 2.** Conceptual representation of how different modelling paradigms enable or restrict the transfer of information between representative volumes. *Left:* A hierarchical FEMxDEM model. It is difficult to model the exchange of particles between representative volume elements, as information must be upscaled to the FEM grid, and then propagated back into a separate DEM simulation. *Middle:* A single scale DEM simulation has no issues with particles moving in space, but requires the simulation of every particle. *Right:* A heterarchical model, which allows direct sub-scale motion between representative volume elements.

are less likely to break. In the paradigm of HGD, there are two contributors to the local arrangement of particles: the porosity and the relative sizes of nearby particles. A particle surrounded by neighbours that are significantly smaller than itself will have a high coordination number and many contacts, and be unlikely to break. A particle with neighbours much larger than itself will typically not contribute to the stress network, and will also be unlikely to break. Only particles with a neighbourhood of similarly sized grains will be likely to break.

The concept of a “neighbourhood” that is local to a particle is a signature of information below the representative volume element level. In the heterarchical paradigm, this information is accessed via the local arrangement of particles along the microstructural coordinate, for example by defining the local average grainsize as

$$\bar{s}_{i,j,k}^{\text{local}} = \frac{1}{2} (s_{i,j,k-1} + s_{i,j,k+1}), \quad (4)$$

where we use the term *grainsize* to indicate a continuous variable that describes the grain size, such as described in [13]. Models have been developed using this idea to simulate the breakage of assemblies of particles, see [8, 9]. In [14], a link was made between this local information and a continuum homogenisation, by upscaling not just the grain size distribution, but also the local average neighbour size distribution. With such a two-dimensional joint size distribution, it was possible to recover an analytic expression for the evolution of the system subject to particle breakage.

### 3.1.2 Growth/agglomeration/nucleation/attrition

Other mechanisms of particle size change can be added to this modelling paradigm. To date, however, these have not been attempted. There is an exhaustive literature in relation to population balance models [15] which outlines the

mathematical formulation and properties of such mechanisms. In fact, the two-dimensional joint size distribution for the breakage mechanism above has been shown to give a population balance model [14]. We expect agglomeration to be implemented similarly to breakage, but with size increase instead of decrease. Nucleation would result as a function of environmental conditions, with a chemical potential carried in the void spaces. Growth and attrition could in principle be added as mechanisms where the size changes continuously as a function of environmental factors.

## 3.2 Open systems

In contrast to the breakage mechanism described above, open systems allow for material and information to pass between representative volumes. The heterarchical modelling paradigm allows for the direct transfer of this information, see Figure 2. Here, we describe three mechanisms of such motion.

### 3.2.1 Void migration

When a dense granular material is deformed, the motion of the particles is controlled by the fact that there must be free space for particles to move into. In the context of HGD, where the solid and void phases are conveniently separated, we can progress in time steps of size  $\Delta t$  and describe probabilities  $P$  that constrain the motion of the solid phase to behave as a granular medium. Several models exist in the literature which stochastically update the location of the solids by swapping their locations with a nearby void, *e.g.*, [16–18]. At this stage we do not constrain the choice of these probabilities except to note that they should be (1) based on our understanding of the motion of granular media, and (2) be relatively simple, and follow the structure shown in Figure 3. For particles to advect with a velocity  $u$ , a distance  $\Delta y$ , in a timestep  $\Delta t$ , we would choose an average probability of advection  $\bar{P}_{\text{adv}}$ ,

$$\overline{P_{adv}} = u \frac{\Delta t}{\Delta y}. \quad (5)$$

### 3.2.2 Segregation

Granular media have a strong tendency to segregate by size, density or other material property when deformed, see *e.g.*, [21]. There is significant ongoing research into the causes and nature of the underlying mechanisms by which segregation occurs, see [22–24] for three recent reviews of the topic. Here, we take a simple approach and state that segregation occurs when voids swap with particles. In reference to Figure 3, this is implemented by requiring that both  $P_{adv}$  and  $P_{diff}$  are size dependent. For segregation, we perturb the typical probability as

$$P_{adv} = \overline{P_{adv}} \cdot \frac{\overline{s^{-1}}}{s}, \quad (6)$$

with  $\overline{s^{-1}}$  the hyperbolic mean grain size. This scaling recovers the expected segregation velocities from [25].

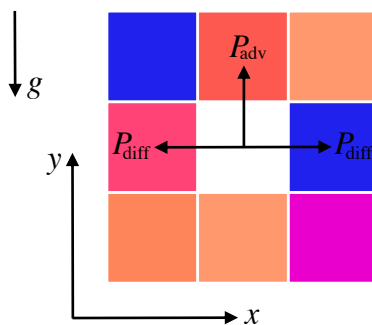
### 3.2.3 Mixing

Complementary to the segregation mechanism is mixing, which causes imperfect segregation, and which is generally considered to be due to collisions between particles. DEM modelling indicates that the diffusivity depends on the particle size and the inertial number [26]. In the context of HGD, this diffusivity arises from diffusive probability  $P_{diff}$ . We model a diffusivity of the form

$$D = \alpha us, \quad (7)$$

which has been observed in several experiments in the discharge of a silo [27, 28]. The parameter  $\alpha$  sets the inverse of the Péclet number,  $\alpha s$ , and controls the strength of diffusion. This leads to our definition for the diffusivity as

$$P_{diff} = D \frac{\Delta t}{\Delta x^2}. \quad (8)$$



**Figure 3.** Void migration mechanism. Unstable voids (shown in white) within a material move due to two mechanisms. Advection, with a probability of occurrence  $P_{adv}$ , in the direction opposed to any resultant body force (in this case gravity  $g$ ), and diffusion, with probability  $P_{diff}$  orthogonal to the advection.

We can additionally define the bulk diffusivity at a location in space via

$$\overline{P_{diff}} = \alpha u \overline{s} \frac{\Delta t}{\Delta x^2}. \quad (9)$$

### 3.2.4 Continuum upscaling

The stochastic rules above admit deterministic results for arbitrarily large numbers of cells in the microstructural direction,  $M$ . Under these conditions, for low concentrations of excess voids (*i.e.*, where voids do not interact and can be modelled individually), we recover an advection-diffusion equation for the bulk motion of the voids [4], as

$$\frac{\partial n}{\partial t} = \frac{\partial^2}{\partial x^2}(\alpha u \overline{s} n) - \frac{\partial}{\partial y}(un). \quad (10)$$

More complex continuum equations can be developed when considering interacting voids, or the effect of segregation and crushing. Some of these are shown in [4]. When including crushing, and potentially other mechanisms of particle size change, HGD can be viewed as a stochastic solver for a population balance model that describes the evolution of a system that depends not only on the local size distribution, but also the local average neighbour size distribution.

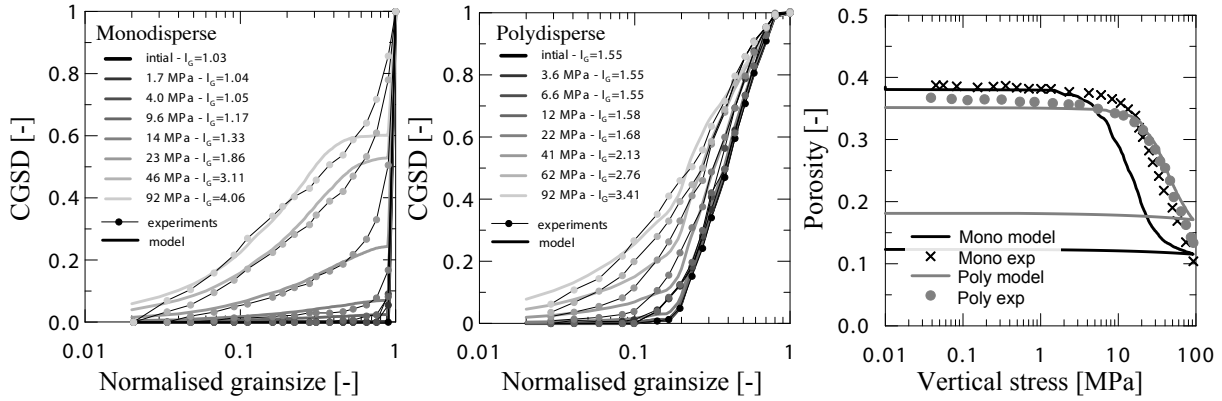
## 3.3 Stability

Particle rearrangement should only occur when the material is in some sense unstable. To date, in existing HGD models, there has been no strong coupling between the stress and the motion of the voids in the material. This has allowed for very simple motion models to be developed, but requires significant simplification and model restriction. In [4], two stability criteria were imposed. The first states that the material is stable if the solid fraction is above a critical value, and the second that the material is unstable if the local gradient of the solid fraction exceeds a threshold value. Between these two criteria, it is possible to model the discharge of a silo that stops with a prescribed angle of repose (set indirectly via the solid fraction gradient).

Future developments should integrate a more robust coupling between stress fields and particle motion. Incorporating dynamic stress-motion feedback remains a key area of ongoing research.

## 4 Applications of Heterarchical Granular Dynamics

HGD has been applied to a variety of granular systems, offering insights into both natural and industrial processes. Below, we list a representative sample of the types of problems that have been modelled to date.



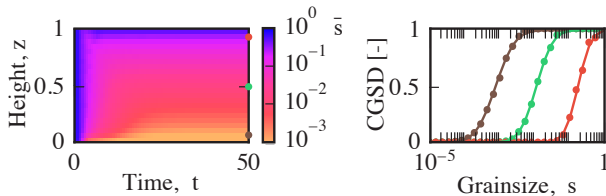
**Figure 4.** HGD model prediction (from [19]) and experimental data (from [20]) for the crushing behaviour of a silica sand undergoing one-dimensional compression. *Left and Middle:* Cumulative grain size distribution (CGSD) for initially monodisperse and polydisperse samples. *Right:* Porosity as a function of vertical stress for both samples.

#### 4.1 Simplified 0D Models

Early studies of HGD focused on simplified zero-dimensional (0D, without considering spatial extent) . In [19], the compression behaviour of crushable silica sand particles was modelled, and compared against experimental data from [20]. As shown in Figure 4, the model produces evolving grain size distributions that vary with initial grain size distribution. For the two cases studied, we predict an evolution not only of the grain size distribution, but also the porosity of the sample.

#### 4.2 1D Models

Several studies have been performed using simplified 1D geometries, looking either at the segregation/mixing/crushing mechanisms in isolation, or coupled together. In Figure 5, we show model output for the case of a 1D granular avalanche with significant particle crushing. In this example, reproduced from [9], an initially uniform grain size distribution is allowed to flow, with a lithostatic stress distribution. During flow, particle crushing occurs, primarily near the base of the flow. The fine particles produced begin to segregate, and an evolving grain size distribution is observed, that has a lognormal distribution. Such

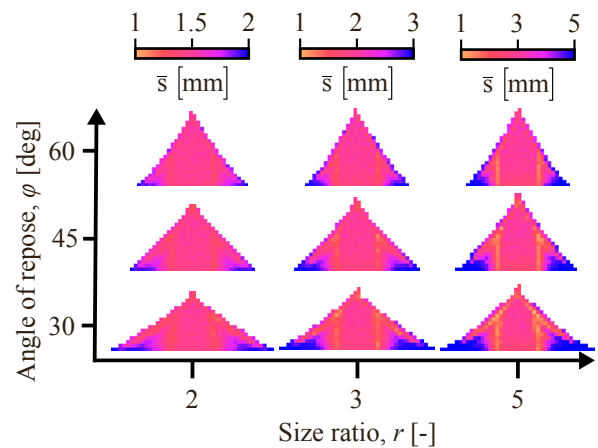


**Figure 5.** A 1D crushable flow with segregation, mixing and comminution from [9]. Initially, the system is homogeneous, and represents a column of grains, homogeneous in the down-slope and cross-slope directions, that evolves over time with a prescribed shear strain rate. *Left:* Spatiotemporal evolution of the average grainsize. *Right:* Cumulative grainsize distribution (CGSD) at three points in the flow, corresponding to the circles on the left. Solid lines are best fit lognormal distributions.

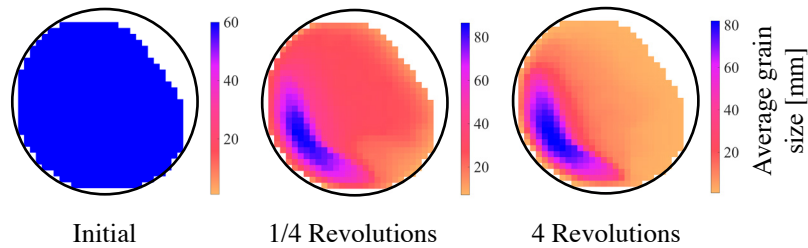
lognormal grain size distributions are observed in several geological deposits, including glacial tills, snow and rock avalanches, debris flows and pyroclastic flows [8].

#### 4.3 2D Models

The first void migration models [16] were formed to describe the discharge of material from silos. The model described here can be used for such cases, and admits discharging velocity fields that closely match those found in experiments, see [4]. In Figure 6, we show several deposits of a rectangular column of material composed of particles of two sizes that has been allowed to quasi-statically collapse under the action of gravity. The final deposit is shown for 9 cases, with three different imposed angles of



**Figure 6.** Column collapse for a bidisperse material with varying angle of repose.  $\phi$  is the imposed angle of repose,  $r$  the size ratio, with the minimum and maximum sizes indicated on the colour bar. Each image corresponds to a map of the average particle size in the final deposit of an initially rectangular mass that has been allowed to collapse under the action of gravity. Based on the model in [4]. Results shown here are not perfectly smooth or symmetric, because only 100 cells are used in the microstructural direction. Figure produced by Dr Shivakumar Athani.



**Figure 7.** Evolution of mean particle size during the simulation of comminution in an AG mill from [10]. The material, initially coarse, is rotated milled by rotation of the container (clockwise), with particles being thrown into the air and landing in the bottom right corner, where most particle crushing occurs, and finer material is produced. Simultaneously, segregation causes large particles to accumulate in the bottom left corner. *Left to Right:* Initial homogeneous state, 0.25 and 4 revolutions.

repose  $\varphi$ , and three size ratios  $r$ . In the future, to model this problem more completely, additional physics should be added to include the motion of material due to inertia to alleviate the implication of quasi-static motion. Additionally, the stability criteria should be revised to appropriately consider the stress fields instead of the geometric argument used currently.

HGD has been extended to model comminution processes in rotary mills, including ball mills, autogenous grinding (AG) and semi-autogenous (SAG) mills in [10, 11]. This application captures the complex interplay of crushing, mixing, and segregation under dynamic flow conditions. The evolution of an initially homogeneous AG mill is shown in Figure 7. In this work, the bulk motion of the material was fixed, and taken either from an analytical model or from coarse grained discrete element simulations.

## 5 The future

Future potential applications of HGD include industrial-scale processes such as large-scale mining operations, pharmaceutical powder handling, agricultural grain sorting, and construction material processing, where traditional DEM faces severe scalability limitations. Compared with DEM simulations, HGD predicts similar grain size evolution and flow patterns, but at significantly reduced computational costs, enabling studies of larger and longer-duration processes.

To enable broad applicability, improvements to HGD should focus on the following:

1. Adding inertia. Currently, it is assumed that particles do not maintain their velocity from one time step to the next.
2. Stress coupling. Stress fields can be calculated via assumption of a particular stress propagation model, whether linear elastic [29], non-linear elastic [30] or more exotic [31].
3. Momentum conservation. Once inertia and stress are defined, momentum can be conserved. This will enable a deeper understanding of the coupling between the stochastic void migration rules and momentum dissipation in the system.

4. Fluid coupling. As HGD provides local measures of the porosity and the grain size distribution, high quality estimates of the local permeability field can be made. Using this permeability, it is possible to predict the flow of fluids through the granular assembly, with a feedback via momentum conservation onto the bulk motion. This would enable a broad variety of boundary value problems to be considered via HGD.

The above improvements could be achieved by extending the probabilities defined in Figure 3 to allow advection and diffusion in arbitrary directions, driven by local force directions. This extension would allow more general force models, such as drag forces from fluids, to be applied.

## 6 Conclusion

HGD has emerged as a powerful framework for modelling and understanding the behaviour of granular materials. To date, HGD has been used to model segregation, mixing and particle crushing in a range of natural and industrial applications. The model is based on stochastic rules of motion which bridge the scales from particle level information to the macro continuum response. Further validation and development are required for this modelling paradigm to be considered ‘general’ in the sense that it can be used for the solution of arbitrary problems, but the work completed to date is indicative that this may be possible in the future. Such future research should focus on extensive validation of HGD against diverse experimental datasets, robust integration of stress-motion coupling, and exploration of adaptive discretisation methods. These steps will solidify HGD as a reliable general-purpose tool for granular material modelling.

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