Chapter 1

Introduction

1.1 Background

Despite being common in everyday experience, granular materials are poorly understood from a theoretical standpoint, and even in the simplest of situations, they can exhibit surprisingly complex behavior. The last twenty years has seen a resurgence of interest in them from the scientific and engineering community, motivated by the possibility that there is new physics to be discovered [59, 60, 10, 64, 34]. Granular materials are frequently viewed in connection with other systems featuring strong confinement (such as glasses and colloids) and thus the central challenges have a much broader applicability.

Granular materials cannot be characterised as a gas, liquid, or solid, and in certain situations, they can exhibit behavior characteristic of each of these three phases [60]. Perhaps some of the most successful work has been in situations where the granular material can be approximated by one of these phases. The behavior of dilute, collisional granular media has been explained using a version of Boltzmann's kinetic theory of gases, modified to account for inelastic collisions [61]. At the opposite limit, the modern methods of soil mechanics, such as Critical State Theory [118, 94], have had some successes in explaining the bulk stresses in a static granular assembly of densely packed particles.

This thesis is primarily concerned with an intermediate regime, of slow flow in

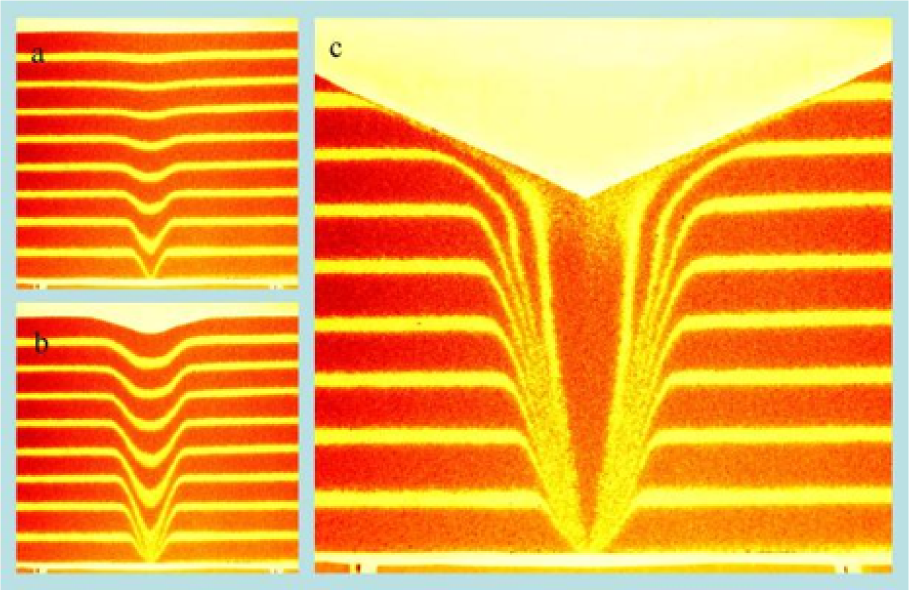

Figure 1-1: Three snapshots of a granular drainage experiment. Red and yellow particles are held between two parallel glass plates and drain from an orifice in the container base. (Samadani and Kudrolli, Clark University.)

dense granular materials. Two everyday examples of this would be drainage of sand in an hourglass, or the flow of seed through a hopper. In these flows, particles form a dense, amorphous packing, and since they interact inelastically, energy is rapidly lost in the system, meaning that individual particles have long-lasting, many-body contacts with their neighbors. Before flow starts, the packing is solid-like and supports stresses, but during flow, the material begins to rearrange and exhibit more liquid-like behavior. The interplay between these two different regimes is poorly understood.

At the microscopic level, particles in a dense granular flow exhibit complex behavior. Experiments have shown that there are large heterogeneities at the level of a single particle [31, 89, 19, 39, 56]. Stresses in granular materials tend not to be evenly distributed, and are often localized along chains of particles, which continually break and reform during flow [57, 139, 138]. This can create challenges for silo design, since the weight of the grains may be focussed on particular points on the silo wall. Even during flow, particles are frequently in long-lasting contact with their neighbors, and thus statistical mechanics approaches are generally invalid, since the system is in an athermal limit, far from equilibrium. Traditional statistical mechanics assumptions, such as particle collisions occurring randomly from a thermal bath, are generally inappropriate due to strong neighbor correlations.

Given the discrete effects at the level of a single particle, one might expect that the flow profiles would exhibit features at this level too, such as cracks or dislocations. However, the macroscopic properties of slow, dense granular flow in most situations are smooth, and are frequently well-approximated by simple functions. Figure 1-1 shows several snapshots from a quasi-2D granular drainage experiment. The flowing region forms a parabola, and using particle image velocimetry, the mean flow in the vertical direction at different cross sections is well-approximated by a Gaussian; similar results have been seen in many other situations [84, 83, 114, 95, 137, 90, 91, 27]. In a rotating Couette shear cell, the velocity profile forms a boundary layer on the rotating wall, with exponential decay into the bulk [80, 87, 72, 21, 88]. In flow down an inclined plane, the velocity profile as a function of height follows an approximately polynomial dependence [107, 7, 18, 123, 126]. In a split-bottom Couette cell, the velocity profiles were well approximated by an error function [45], with the data being accurate enough to tell this apart from a hyperbolic tangent. It is tantalizing to wonder whether the flow in these different geometries can be explained by a single formalism, in the same way that the Navier-Stokes equations can describe a large class of fluid flows in arbitrary geometries. However, the variety of the functional forms, coupled with the lack of a good microscopic model, make the task of finding such a theory challenging. While there have been theories that explain a specific subset of these geometries, there is no well-accepted overreaching theory. The lack of such a theory is a hurdle to industry, where grains and powders are frequently manipulated.

There is perhaps cause to be optimistic that some of these key questions about granular materials may be answered in the near future. The last ten years has seen the development of many theoretical models for granular flow, with an diverse array of physical postulates, such as “granular eddies” [41], granular temperature-dependent viscosity [116], density-dependent viscosity [80, 21] “shear transformation zones” [43, 44, 75, 73, 74], and partial fluidization [8, 9]. None of these models could be considered a general theory, and typically only explain a narrow subset of possible geometries.

However, it may well be that a complete theory incorporates aspects from some of these current ideas.

The wealth of new theories has been coupled with an increase in the sophistication of experimental techniques. While granular materials are tangible, gaining pertinent experimental information about the details of flows poses many challenges. To observe stresses at the level of a particle, experimentalists have made use of photoelastic discs [82]. Another obvious problem in granular experiments is that it is difficult to visualize the bulk flow, although recently several techniques, such as magnetic resonance imaging [88], diffusing-wave spectroscopy [85], confocal microscopy [142], and index-matching with an interstitial fluid [136, 135, 122, 102], have been used to directly measure properties of flow in the bulk.

Simulation of granular materials presents another promising avenue of investigation. In the past five years, with the large scale deployment of parallel computer clusters in universities and research labs, it has become possible to carry out Discrete Element Method (DEM) simulations on a reasonable scale [1, 144, 129, 26, 123, 24, 48]. Although computationally intensive, the DEM simulations offer the ability to investigate many aspects of a granular flow in complete, three-dimensional detail, without any of the experimental difficulties, and they have made a number of important contributions.

1.2 Previous work at MIT before this thesis

Hopper drainage is perhaps one of the simplest examples of a dense granular flow, since it requires no external forcing and happens by gravity only. Over the past forty years, it has been extensively studied, and a number of continuum models [77, 90, 95, 108, 94, 92] have been proposed. However, these models primarily concentrated on the steady state mean flow, and certain practical situations arise in which one may be interested in the behavior of the constituent particles, such as how they mix and rearrange. Perhaps one of the most interesting examples is in the pebble-bed nuclear reactor, a schematic of which is drawn in figure 1-2. In the pebble-bed reactor, fuel is inserted as spherical pebbles, which are slowly and continuously drained through a large cylindrical container. In some designs of reactors, including the one shown here, there are two types of pebbles – a core of reflecting moderator pebbles, surrounded by an annulus of fuel pebbles. For this type of design, diffusion of the fuel/moderator interface has considerable implications for reactor design and safety.

In addition to particle diffusion, some of the functional forms seen in granular flow experiments suggest that the velocity field itself may in part be explained by a diffusing quantity. In particular, the drainage experiments, with a gaussian velocity profile whose width scales according to the square root of height, suggest a solution motivated by a diffusion equation. As discussed in following chapter, this possibility was considered by several authors, who postulated the void model [76, 77, 78, 90, 25]. In this model, voids of free space are introduced at the orifice, and diffuse upwards, causing the particles to move correspondingly downwards. Despite its simplicity, the result has been shown to be in reasonably good agreement with the experimental results.

Motivated by this, Choi, Kudrolli, Rosales, and Bazant [28] carried out one of the first experimental studies of particle diffusion in granular drainage. Their results (summarized in section 2.2) show that the regime of slow, dense granular flow is governed by a distinctly non-thermal picture, where particles undergo long-lasting contacts with their neighbors, and the features of the flow are predominately governed by geometry and packing constraints. In particular, they observed that for a large range of hopper drainage experiments, altering the orifice size resulted in a change in the overall flow rate, but did not alter the geometry of the flow profile – the flow velocities were scaled by a constant factor. The amount of diffusion observed was very small, with the length scale of particle diffusion being two to three orders of magnitude smaller than the length scale associated with the overall width of the flow.

A natural next step is to ask whether these results could be explained by a mathematical model, and perhaps the only candidate in the literature is the void description. While originally proposed to explain the mean flow, the void model also gives a microscopic model for particle motion, which was not considered by the original authors.

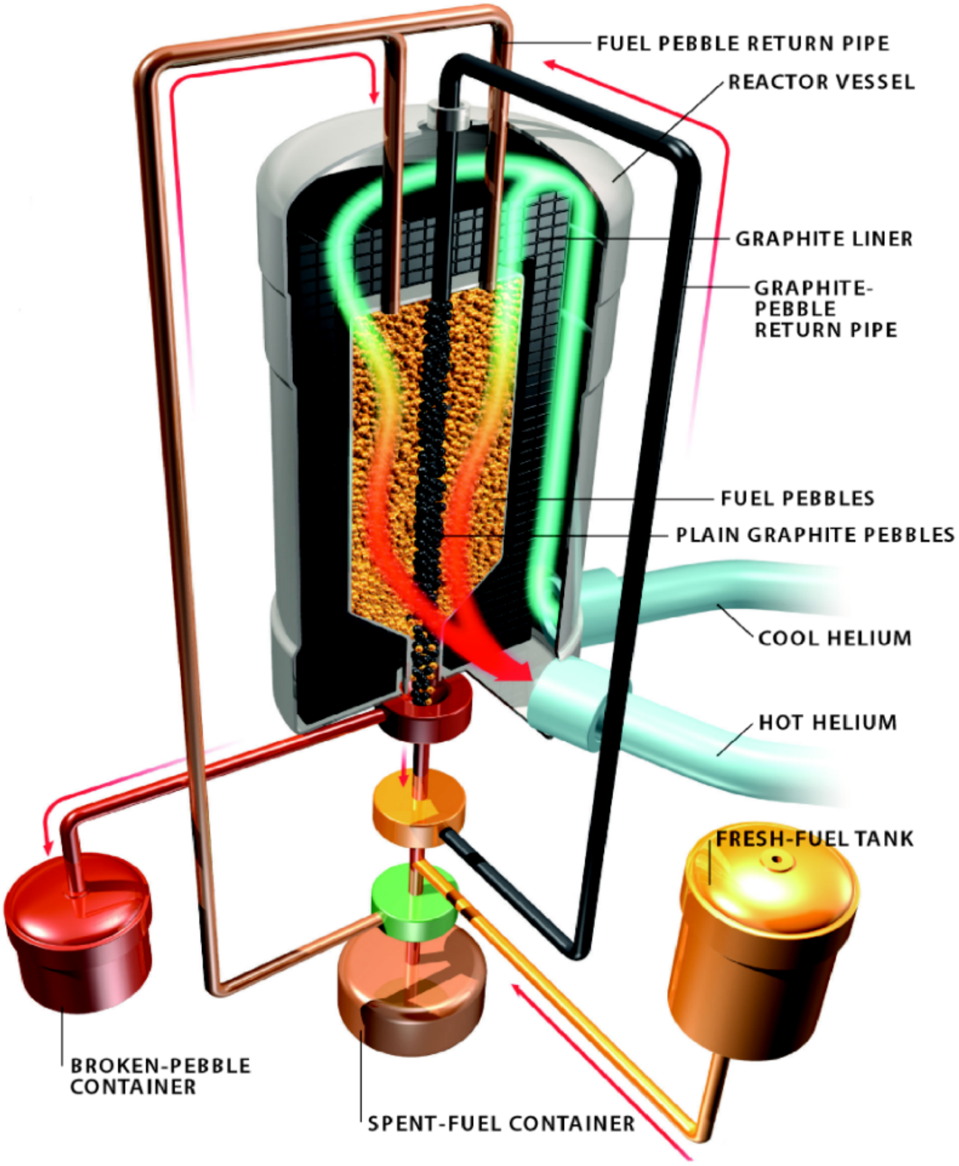

Figure 1-2: A schematic diagram of the pebble-bed nuclear reactor. The evolution of the interface between the two types of particles is critical to the reactor design.

However, despite its successes with the mean flow, the void model greatly overpredicts the amount of particle diffusion, since the length scale of particle diffusion is the same as the diffusive length scale of the flow profile. One of the main deficiencies of the void model is that it does not respect the packing geometry of the granular material: it allows individual particles to move independently of the rest of the packing, but in reality, a single particle may be strongly constrained by its neighbors.

Based on this idea, Bazant proposed the spot model [17] which provides a more realistic microscopic mechanism for particle motion, by moving particles in local groups, corresponding to the fact that they must move co-operatively. The spot model predicts similar mean flows to the void model, but reduces the particle diffusion by several orders of magnitude, consistent with the experimental evidence. It remains simple enough for mathematical analysis, and makes a number of physical predictions. While a complete flow may be made up of many spots, and thus a single spot cannot be directly observed, the theory predicts that spots would cause local, spatial velocity correlations. These were subsequently found by Choi in the granular drainage experiments, providing a validation of the theory.

The spot model also forms the basis of a simulation technique. Choi carried out two dimensional spot model simulations, which were able to capture many aspects of the flow in the hopper experiments, such as the velocity profiles. However, these preliminary simulations had one large flaw: even though the movements of an individual tracer particle appear physically reasonable, the packing arrangements that were generated would exhibit overlapping particles, particularly in regions of high shear. This became referred to as the "density problem". Several simple modifications to the spot model were investigated, such as the use of persistent random walks [55], spot rotations, or extra particle diffusion, and while these led improvements in the, none were successful in creating fully valid particle packings.

1.3 The contribution of this thesis

During the past decade, scientific computation has become increasingly important in applied mathematics, providing insight into many problems that would preclude a simple analytical description. Since granular materials exhibit a complicated interplay between discrete effects at the particle level, and continuum effects and a macroscopic level, they are ideally suited to being studied by computer. At the most general level, this thesis has made use applied computational methods from a variety of different perspectives to examine aspects of granular flow that would be difficult to address in either pure theory or experiment.

1.3.1 Discrete Element Simulation

While Choi was able to show the existence of velocity correlations in experiment, the results had a fundamental drawback that the measurements could only be taken of the particles which were pressed against the front and back walls of the silo, as there was no direct way to imaging the particle rearrangements in the bulk of the flow. As mentioned above, experimental techniques have been developed to probe into the bulk of the granular flow, but these usually provide limited information, and are unsuitable for this case where we would like to know in detail about microscopic rearrangements of the individual particles.

DEM simulation provides an ideal tool for this situation, since it gives complete information about all particles in a granular flow. Using a parallel discrete element code developed at Sandia National Laboratories (discussed in section 2.6), the author ran a full-size simulation of Choi's experimental geometry. With no fitting, the computed velocity profiles matched Choi's experimental results to a high degree of accuracy (section 2.7). Computing the velocity correlations at the surface of the packing yielded similar results to Choi's experiment. However, in the DEM simulation, it was possible to show that velocity correlations were also present in the bulk of the granular flow, validating the use of the spot model in fully three-dimensional granular packings.

1.3.2 Solution to the “density problem”

In addition to carrying out the large-scale DEM simulations above, the author also created a three-dimensional spot simulation of granular drainage. Initial studies of the spot model showed that the density problem was still present in three dimensions. However, the author demonstrated that it could be eliminated by modifying the spot model (discussed in chapter 3) to incorporate an elastic relaxation step, whereby after the bulk spot displacement, any overlapping particles experienced a small repulsion. Surprisingly, it was found that only a small, single-step correction was required to generate non-overlapping packings, and that the addition of this did not significantly alter any of the other aspects of the simulation. The author used this model as a basis for a multiscale simulation of granular drainage that matched many aspects of a corresponding Discrete Element simulation. Since the spot simulation suppresses much of the details of individual particle contacts, and concentrates on the packing geometry only, it required approximately a hundredth of the computational power of DEM, making it a promising technique for applications where one wishes to rapidly gain approximate answers about granular drainage problems.

1.3.3 How do random packings flow?

Random packings have received much attention in the literature, but most of the work has concentrated on the geometry of static assemblies [132, 81, 133, 36], with much of the current work focusing on the jamming transition [134, 99, 100, 37, 79]. However, little attention has been paid to how a random packing of particles will rearrange during flow. One of the most surprising results of the above simulations was that the spot model was able to recreate and track several important signatures of the random packing structure that were seen in DEM. The spot model with relaxation can be viewed as one of the first theoretical models of particle rearrangement in a flowing random packing, and an in-depth study of its stability was carried out. By moving spots around in a periodic box [104] the algorithm can also be used as a method of generating static random packings.

1.3.4 Additional studies of the spot model

Chapter 4 continues with several extensions to the basic spot model. Since spots are thought of as carrying free volume, it is interesting to track and compare the distribution of free space in the two simulations, and some important differences were observed. Carrying this out required the author to construct a three-dimensional Voronoi tessellation algorithm which is described in detail. Also in this chapter, two alternative spot models were considered, to investigate whether the simulation could accurately describe the free surface, and see whether it would work in a two dimensional crystalline flow. Finally, since the spot influence is local, it lends itself well to running on a parallel computer, and two different parallelization schemes were considered.

1.3.5 A simulation study of the pebble-bed reactor geometry

Concurrent with the spot simulation described above, the author carried out an detailed study of granular flow in a pebble-bed nuclear reactor, described in chapter 5. In collaboration with Sandia National Laboratories, several full-size DEM simulations of pebble-bed reactors were carried out, based on the MIT Modular Pebble Bed Reactor (MPBR) [130, 2] design. Unlike the spot model simulations, this study was primarily focused on asking questions of relevance to engineering, such as the residence-time distribution of pebbles draining through the reactor, although many of the results complemented the spot model studies described in other chapters. In addition to the full-size runs, several half-size simulations were carried out to look at the influence of wall friction, and to investigate the feasibility of a bidisperse pebble-bed reactor core.

1.3.6 A general model of dense granular flow

Despite the spot model's successes, it was unclear how to extend it to other geometries to form a general multiscale simulation technique. The notion of diffusing free volume seems very specific to granular drainage. However, Kamrin and Bazant [65, 66] found a method of relating the spot motion to granular stresses, and were able to extend the applicability to several other geometries, including the Couette shear cell. In chapter 6 we carried out an in-depth test of the SFR to DEM simulations in both the silo and Couette geometries, making the SFR one of the first theoretical models to describe two types of geometry using the same formalism.

1.3.7 Measuring a granular continuum element

Despite the SFR's successes, the description of stresses that it made use of had several troubling features, and we wished to test these directly. However, given the complications of force chains at the local level, it was unclear whether there was any notion of a continuum stress at the particle level. In chapter 7 it was shown that stress, and other material quantities can be interpreted in an approximate sense at the spot scale even though they would be intractable at the level of a a single particle. By carrying out a variety of DEM simulations, and viewing the results as an ensemble of "granular elements" at the spot scale, it was possible to directly test the assumptions of Mohr-Coulomb plasticity at the local level.