

Multi-scale multiphase modelling of granular flows



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I would like to dedicate this thesis to my loving parents

Declaration

I hereby declare that except where specific reference is made to the work of others, the contents of this dissertation are original and have not been submitted in whole or in part for consideration for any other degree or qualification in this, or any other university. This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration, except where specifically indicated in the text. This dissertation contains fewer than 65,000 words including appendices, bibliography, footnotes, tables and equations and has fewer than 150 figures.

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Abstract

Geophysical hazards usually involve multiphase flow of dense granular solids and water. Understanding the mechanics of granular flow is of particular importance in predicting the run-out behaviour of debris flows. The dynamics of a homogeneous granular flow involve three distinct scales: the microscopic scale, the meso-scale, and the macroscopic scale. Conventionally, granular flows are modelled as a continuum because they exhibit many collective phenomena. Recent studies, however, suggest that a continuum law may be unable to capture the effect of inhomogeneities at the grain scale level, such as orientation of force chains, which are micro-structural effects. Discrete element methods (DEM) are capable of simulating these micro-structural effects, however they are computationally expensive. In the present study, a multi-scale approach is adopted, using both DEM and continuum techniques, to better understand the rheology of granular flows and the limitations of continuum models.

The collapse of a granular column on a horizontal surface is a simple case of granular flow; however, a proper model that describes the flow dynamics is still lacking. In the present study, the generalised interpolation material point method (GIMPM), a hybrid Eulerian – Lagrangian approach, is implemented with the Mohr-Coloumb failure criterion to describe the continuum behaviour of granular flows. The granular column collapse is also simulated using DEM to understand the micro-mechanics of the flow. The limitations of MPM in modelling the flow dynamics are studied by inspecting the energy dissipation mechanisms. The lack of collisional dissipation in the Mohr-Coloumb model results in longer run-out distances for granular flows in dilute regimes (where the mean pressure is low). However, the model is able to capture the rheology of dense granular flows, such as the run-out evolution of slopes subjected to lateral excitation, where the inertial number $I < 0.1$.

The initiation and propagation of submarine flows depend mainly on the slope, density, and quantity of the material destabilised. Certain macroscopic models are able to capture simple mechanical behaviours, however the complex physical mechanisms that occur at the grain scale, such as hydrodynamic instabilities and formation of clusters, have largely been ignored. In order to describe the mechanism of submarine granular flows, it is important to consider both the dynamics of the solid phase and the role of the ambient fluid. In the present study, a two-dimensional coupled Lattice Boltzmann LBM – DEM technique is developed

to understand the micro-scale rheology of granular flows in fluid. Parametric analyses are performed to assess the influence of initial configuration, permeability, and slope of the inclined plane on the flow. The effect of hydrodynamic forces on the run-out evolution is analysed by comparing the energy dissipation and flow evolution between dry and immersed conditions.

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Nomenclature

Roman Symbols

- a** Acceleration of a grain or a material point
- a* Initial aspect ratio of a granular column
- b** Body force
- c* Concentration in Kinetic theory (or) Pressure wave velocity
- d* Grain diameter
- E* Energy
- e* Void ratio of the sample
- E_D Energy lost through drag
- E_f Energy lost through friction
- E_k Kinetic energy
- E_p Potential energy
- E_r Energy lost due to remolding and transformation
- E_v Energy lost through viscous dissipation
- f / F** Applied force
- G* Gradient of the function (or) Shear modulus
- g* Acceleration due to gravity
- K* Bulk modulus

H	Height of a granular column
h	Vertical length scale in shallow water approximation
I	Inertial number (or) Moment of Inertia
k	Stiffness of a grain (or) time step
k_f	Dimensionless parameter defined as the ratio of normal stiffness k_n to the applied normal pressure σ'_n
k^*	Dimensionless parameter defined as the ratio of elastic to inertial effects
L	Length of a granular column (or) background cell size
l	Horizontal length scale in shallow water approximation (or) particle spacing in the Material Point Method
m	Mass of a granular column
N	Shape function or Number of grains/material points
p	Pressure
R	Radius of a grain in DEM
r	Radius or hydrodynamic radius of a grain in LBM
T	Temperature
t	Time
u	Velocity component along x -direction
V	Volume of a material point
v	Velocity component along y -direction
W	Width of the channel
w	Weight function / test function
p	Position of a material point / node

Greek Symbols

α	Conductivity
χ	Characteristic function
δ	Overlap between grains (or) Dirac function
ε	Coefficient of restitution
ε	Strain component
η_h	Packing density, defined as the ratio of volume of solids to the total volume (V_s/V)
Γ	Dissipation through inelastic collision
γ	Viscous damping of a grain
$\dot{\gamma}$	Shear rate
λ	Constant of proportionality in the power-law relationship
μ	Coefficient of friction
Ω	Domain under consideration
ω	angular velocity of a grain
ϕ	Friction angle in degrees
φ	angular orientation of a grain
$\bar{\phi}$	Weighting function
ρ	Density
σ	Stress or confining pressure
τ	Shear stress (or) Surface traction
τ_c	Critical time
θ	Slope angle

Superscripts

' Effective component of the normal stress

Subscripts

0	Initial state
ext	External
f	Final state
i	Property of the computational node (MPM) or grain (DEM)
int	Internal
max	Maximum
min	Minimum
n	Normal component
p	Property of the material point
t	Tangential component

Chapter 1

Granular flows

1.1 Introduction

A granular material is a conglomeration of a large number of discrete solid grains of sizes greater than $1\mu m$ whose behaviour is governed by frictional contacts and inelastic collisions. A schematic representation of the size range of the granular materials is presented in figure 1.1. Granular materials, characterized by the interaction between individual grains, lie between two extremes scales: the molecular-scale range predominated by the electrostatic force, i.e. Van der Waals forces, and the continuum scale which is described by the bulk property of the material. In various soil classification systems, sand is classified as a granular material having grain sizes greater than $75\mu m$. A grain size of $75\mu m$ is an important transition point, where the frictional effect starts to dominate the material behaviour and the effect of the electrostatic Van der Waals forces diminishes. The extent of the grain size range of the granular materials from the molecular size to a continuum scale indicates that they have a complex behaviour, demonstrating a mix of grain-like and continuum-like behaviour.

The physics of non-cohesive granular assemblies is intriguing. Despite being ubiquitous in nature and having a wide range of applications including geo-hazard predictions, granular materials are the most poorly understood materials from a theoretical standpoint. For years, granular materials have resisted theoretical development, demonstrating non-trivial behaviour that resembles solid and/or fluid-like behaviour under different circumstances. Even in the simplest of situations, granular materials can exhibit surprisingly complex behaviour. Macroscopically, the complex mix of solid and fluid-like behaviour can be illustrated by a simple example; while one walks on the beach, the solid-like behaviour of soil becomes evident as it supports one's weight, but if we scoop a handful of soil and allow it to run through the fingers, the fluid-like nature becomes obvious.

Microscopically this complex behaviour has various reasons. The range of the grain size gives rise to complex interactions between grains constituting the granular media. Unlike other micro-scale particles, soil grains are insensitive to thermal energy dissipation (Mehta, 2011), because the thermal energy dissipation in a granular material is several orders of magnitude smaller in comparison with the energy dissipation due to interaction between the grains. The thermal energy scales are small when compared to the energy required to move the grains. The granular material reaches the static equilibrium quickly due to its dissipative nature, unless an external source of energy is constantly applied (Choi, 2005).

Our knowledge of the behaviour of granular assemblies is restricted to two extremes: the solid-like behaviour of dense granular assemblies that resist the shearing force by undergoing plastic deformations, and the fluid-like flow behaviour characterized by high shear rates. Granular media are *a priori* simple systems made of solid grains interacting through their contacts. However, they still resist our understanding and no theoretical framework is available to describe their behaviour (Pouliquen et al., 2006). The strong dependency of the behaviour of granular material on its surrounding environment makes it difficult to have a unified theoretical framework. When strongly agitated, the granular material behaves like a dissipative gas, and kinetic theories have been developed to describe this regime (Popken and Cleary, 1999; Xu et al., 2003). On the other hand, during slow deformations, the quasi-static regime is dominated by steric hindrance and friction forces are often described using plasticity theories. In between the two regimes, the material flows like a fluid, and the grains experience enduring contacts, which is incompatible with the assumptions of the kinetic theory (Pouliquen et al., 2006) that describes the dilute regime of a granular flow. Typical granular flows are dense and hence a fundamental statistical theory is not appropriate to describe their properties. Moreover, during the process of granular flow, the material can exist in all the above-mentioned states, which further complicates our understanding of granular flows.

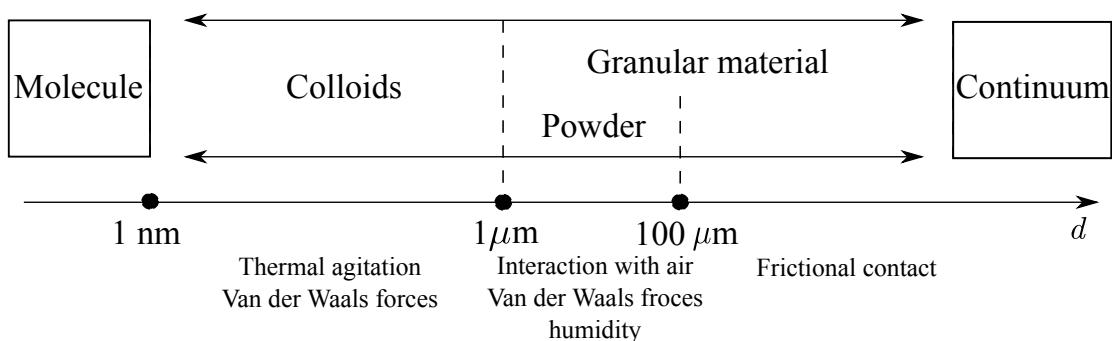


Figure 1.1 Particle size range and their predominant characteristics

1.2 Modelling granular flow

Different approaches have been used to model granular flows at different scales of description. The dynamics of a homogeneous granular flow involve at least three distinct scales: (1) the *microscopic scale* characterized by small time and length scales representing contact/grain interactions, (2) the *mesoscopic scale*, where grain rearrangements, development of micro-structures and shear rates have a dominant influence on the granular flow behaviour, and (3) the *macroscopic scale* which involves large length scales that are related to geometric correlations at even larger scales. The interesting issue is whether one should consider or neglect a particular scale while modelling the granular dynamics (Radjai and Richefeu, 2009). However, the difficulty in modelling the granular flows originates from the fundamental characteristics of the granular matter such as negligible thermal fluctuations, highly-dissipative interactions, and a lack of separation between the microscopic grain scale and the macroscopic scale of the flow (Goldhirsch, 2003).

Granular flows display a large span of grain concentrations and therefore exhibit different behaviour at different concentrations (figure 1.2). Granular flows can be classified into three different regimes (Jaeger et al., 1996): (a) in the dilute part of the flow, grains randomly fluctuate and translate, this form of viscous dissipation and stress is named as the *kinetic regime*. This regime is characterized by grains moving freely between successive collisions (Goldhirsch, 2003). (b) at higher concentration, in addition to the previous dissipation form, grains can collide shortly, this gives rise to further dissipation and stress, called as the *collisional regime*. This intermediate fluid-like regime is dense but still flows like a fluid and the grains interact both by collision and through friction (Midi, 2004; Pouliquen and Forterre, 2002). Transfer of grain kinetic energy and momentum within a rapidly flowing granular medium occurs during these collisions (Popken and Cleary, 1999). (c) at very high concentration (more than 50% in volume), grains start to endure long, sliding and rubbing contacts, which gives rise to a totally different from of dissipation and stress, *frictional regime*. This dense slow quasi-static regime is characterized by long duration between contacts and grain interaction via frictional contact (Roux and Combe, 2002).

The momentum and energy transfer will be different according to the granular regimes. For the granular phase, it is clear that any mathematical model attempting to model the granular flow must account for the above mechanisms, at any time and anywhere within the flow. The mathematical models require a comprehensive unified stress tensor able to adequately describe stress within the flow for any of these regimes, and this without imposing what regime will dominate over the others. Several theoretical frameworks have been used to describe the granular flow behaviour. Frictional behaviour predominates in most granular flows. Hence, continuum models based frictional properties of the granular mass have been

widely adopted to discuss the granular flow behaviour. Alternatively, dilute granular flow behaviour is conventionally modelled using the kinetic theory, while the dense granular flows are described using the $\mu(I)$ rheology. In certain conditions, where the lateral extent of the flow is significantly larger than the vertical component, shallow-water approximation is used. The capability and limitation of the various frameworks are discussed below.

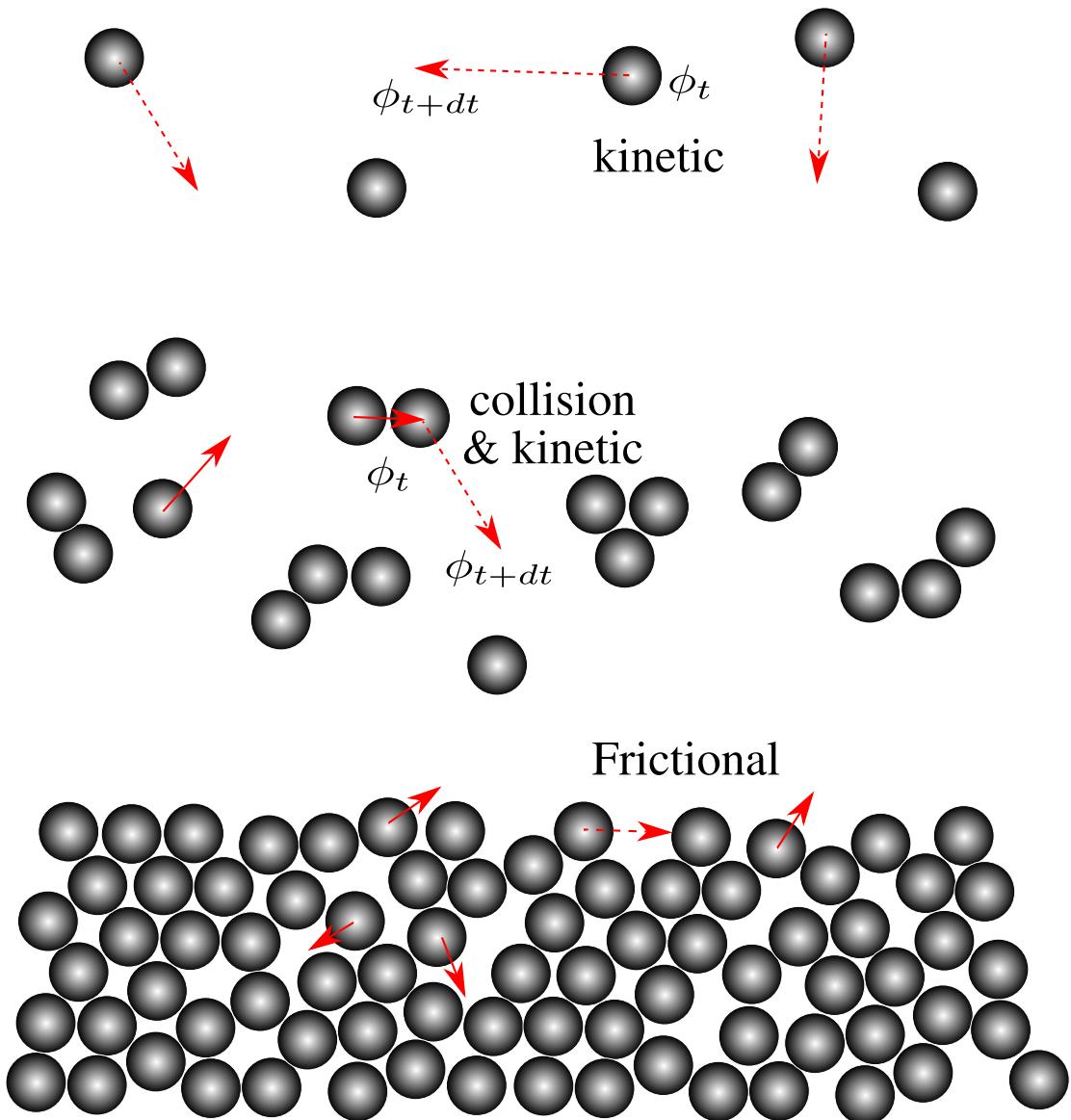


Figure 1.2 The modes of viscous dissipation in a granular flow

1.2.1 Continuum models

In the frictional regime, grains experience long and permanent contacts when they rub and roll against each other. Hence a stress tensor based on the mechanical law of friction must be developed. Granular flow modelling began as early as 1776 with Coulomb's paper describing the yielding of granular material as a frictional process. Although it was not about granular flows, *per se*, the prediction of soil failure for civil engineering applications describes the onset of structural collapse leading to catastrophe (Campbell, 2006). Mohr-Coulomb's yield criterion along with a flow rule from metal plasticity is sufficient to describe the behaviour of granular flow as a continuum process, without considering the interaction of individual grains.

Advanced models based on the critical state concept (Schofield and Wroth, 1968) provide further insight into continuum description of granular flows. According to critical state theory, the 'under consolidated' or loose soil tends to increase in density upon shearing, while the dense 'over consolidated' soil dilates when sheared, until it reaches the critical state. As dense granular flow involves large shear stresses, it is reasonable to assume that the shearing occurs at the critical state. Large applied stress can cause the granular solids to deform at the grain scale and squeeze them into the inter-grain pores. Granular flows experience rapid shearing and is therefore reasonable to assume that the flow is incompressible and takes place at the critical state (Campbell, 2006).

The main limitation of the continuum approach is the assumption that the friction angle, ϕ , is a constant material parameter (Potapov and Campbell, 1996). Although the mechanism of dense granular flow is attributed to bulk friction, it is the formation of force chains and the rearrangement of internal structure of the granular assembly that causes friction-like behaviour. Experiments (Savage and Sayed, 1984; Savage, 1984) and computer simulations (Campbell and Brennan, 1985) indicate a weak relation between the bulk friction and the packing density, due to the micro-structural rearrangement of grains (Campbell, 1986). As the packing density increases, the grains tend to arrange themselves in a regular order when sheared. In order to understand the development of micro-structure, it is important to look at the grain-level interactions. Bagnold (1954) was the first to try and model granular materials as individual grains. Bagnold's theory of motion of individual grains in a shear flow and inter-grain friction inducing random velocities is reminiscent of the thermal motion of molecules in the kinetic theory of gases.

1.2.2 Kinetic theory

The kinetic theory of gases assumes that the particles interact by instantaneous collisions, which implies only binary (two-particle) collisions. The interactions are modelled using a single coefficient of restitution, to represent the energy dissipated by the impact normal to the point of contact between the interactions, and for the most part, the surface friction or any other particle interactions tangential to the point of contact are ignored (Campbell, 1990). Jenkins and Savage (1983) extended kinetic theory for thermal fluids to idealized granular mixtures to predict the rapid deformation of granular material by including energy dissipation during collision for nearly inelastic particles. Savage and Jeffrey (1981) extended the kinetic theory to predict simple shear flow behaviour for a wide range of coefficients of restitution. Kinetic theory is capable of predicting the shear flow behaviour only for mixtures composed of particles with identical density and size (Iddir and Arastoopour, 2005), however real systems are composed of particles that vary in size, and segregation of particles can occur.

The formulation of gas kinetic theory can be used to derive a set of equations for granular flow if the particles are assumed to be rigid. In turn, the rigid particle assumption implies that all contacts occur instantaneously. Thus, there is vanishing probability of multiple simultaneous contacts and only binary contacts are considered. From there, kinetic theory formulation yields a set of Navier – Stokes like equations. Conservation of mass is written as

$$\frac{d\rho c}{dt} + \rho c \nabla \cdot \mathbf{u} = 0. \quad (1.1)$$

Conservation of momentum

$$\rho c \frac{d\mathbf{u}}{dt} = \nabla p(\rho, c, T, \varepsilon) + \nabla \cdot (\eta(p, \rho, c, T, \varepsilon) \nabla \mathbf{u}). \quad (1.2)$$

Conservation of granular energy (granular temperature)

$$\rho c \frac{dT}{dt} = \nabla \cdot (\alpha(p, \rho, c, T, \varepsilon) \nabla T) + \tau : \nabla \mathbf{u} - \Gamma(p, \rho, c, T, \varepsilon). \quad (1.3)$$

where α is the conductivity, $\tau : \nabla \mathbf{u}$ is the temperature production by shear work, p is the pressure, concentration is c , ρ is the density, ε is the coefficient of restitution, T is the granular temperature and Γ is the dissipation through inelastic collisions. There are several problems that should be immediately apparent with this formulation. The most obvious is that the range of applicability of rapid flow theory is limited. The solid phase stresses are viscous in nature (eq. 1.2), which results in a no-force condition when the granular mass is static (Campbell, 2006).

Kinetic theory is valid for dispersed granular flows (Ng et al., 2008). Van Wachem et al. (2001) observed that numerical simulations of dense granular flow based on kinetic theory did not accurately capture experimental data on fluidised bed expansion. Confined granular flows are usually dense, because of their mechanism of energy dissipation and their tendency to form clusters. Dense granular flows lie in an intermediate regime, where both the grain inertia and the contact network have significant influence on the flow behaviour (Pouliquen and Forterre, 2002). Thus, a part of the force is transmitted through the force network, which contradicts the two basic assumptions in the kinetic theory, i.e. binary collision and the molecular chaos.

For dense granular flow conditions, the total stress transmission in the flow regime is the sum of the rate-dependent (collision-transition) and the rate-independent (friction) components (Ng et al., 2008). Addition of a frictional stress component (Schaeffer, 1987) to kinetic theory improves the ability of the model to predict the dense granular flows. The main advantage of kinetic theories is that they can be used to derive deterministic constitutive laws to describe the behaviour of granular flows in a theoretical framework (Jenkins and Savage, 1983). Kinetic theories formulated on the assumption that the solid phase stress has a viscous response have limitations when applied to granular flows. A viscous material produces no force unless it is in motion, hence kinetic theory based on viscous solid phase cannot explain the static force exerted by the granular materials on the walls, as observed in experiments. The frictional component that is based on long-duration contact is added to the instantaneous collision contacts term, which is self-contradictory. Also, the rapid-flow models based on gas kinetic theory assume that the molecular collisions are elastic, which means that they do not dissipate energy (Campbell, 2006), which is in contrast to the reality. Finally, the important assumption of gas kinetic theory is molecular chaos, which assumes no correlation between the velocities or positions of the colliding particles, which is not true especially in a dense granular flow where the particles interact many times with their neighbours and a strong correlation between their velocities is inevitable.

1.2.3 Rheology

Rheology is the science of flow of materials with solid and fluid characteristics. In practice, rheology is principally concerned with describing the mechanical behaviour of those materials that cannot be described by the classical theories, by establishing an empirical relation between deformation and stresses. Consider a granular assembly of grains having diameter d and density ρ_d under a confining pressure σ'_n (see figure 1.3). Assume the material is sheared at a constant shear rate, $\dot{\gamma} = v_w/L$, imposed by the relative movement of the top plate with a velocity v_w . In the absence of gravity, force balance implies that the shear stress, $\tau = \sigma_{xy}$,

and the normal stress, $\sigma'_n = \sigma_{xy}$, are homogeneous across the cell. This configuration is the simplest configuration to study the rheology of granular flow, i.e. to study the effect of strain rate, $\dot{\gamma}$, and pressure, σ'_n on the volume and shear stress, τ .

Even though the granular materials have been extensively researched at microscopic level, the continuum representation of granular materials in terms of conservation of mass and momentum is still an area of concern (Daniel et al., 2007; Midi, 2004). The prediction of rheology of granular materials even in the simplest case is complicated as they exhibit rate-dependent behaviour and no single constitutive equation is able to describe the behaviour over a range of shear stress rates. Da Cruz et al. (2005) developed a well known rheology for granular flows, that is based on simple two-dimensional shear in the absence of gravity and establishes that the flow regime and rheological parameters scale with a dimensionless number that represents the relative strength of inertia forces with respect to the confining pressure (Daniel et al., 2007), along the lines of Savage and Hutter (1991). The shear stress, τ , is proportional to the confining pressure, σ'_n , and is written as

$$\tau = \sigma'_n \mu(I). \quad (1.4)$$

The friction coefficient μ depends on the single non-dimensional parameter I , expressed as

$$I = \frac{\dot{\gamma}d}{\sqrt{\sigma'_n \rho_p}}. \quad (1.5)$$

The parameter I can be interpreted in terms of different time scales controlling the grain flow. If the grains are rigid, i.e. neglecting the elastic properties of the grains, then I is the only non-dimensional parameter in the problem. Hence, the shear stress, τ , has to be proportional to the pressure, σ'_n , times a function of I . Comparing the shape of the function $\mu(I)$ with the experimental results of flow down an inclined plane, Jop et al. (2006) observed that the frictional coefficient increases from a minimal value of μ_s to an asymptotic value of μ_2 , when the value of I increases. The variation of friction coefficient with I is shown in figure 1.4. The friction coefficient can be related to the inertial number I as

$$\mu(I) = \mu_s + \frac{\mu_2 - \mu_s}{I_o/I + 1}, \quad (1.6)$$

where I_o is constant, typically in the range of 0.25 - 0.3.

To formulate a complete constitutive model, it is essential to describe the volumetric behaviour. Based on dimensional analysis, it can be argued that the volume change is also a function of dimensionless parameter I and that it also depends on the maximum and the minimum possible void ratios and the time for microscopic rearrangement of grains.

Consider two rows of mono-dispersed grains. When a grain is located in the gap formed by two adjacent grains, it is assumed to have a maximum packing fraction. As the grain is sheared along the bottom row of grains, it moves out of the gap resulting in a minimum packing fraction. The duration required for this rearrangement is directly proportional to the volume fraction. The dimensionless shear rate, expressed as the ratio between the duration of re-arrangement to the mean duration (see figure 1.18), has a linear relationship with the volume fraction.

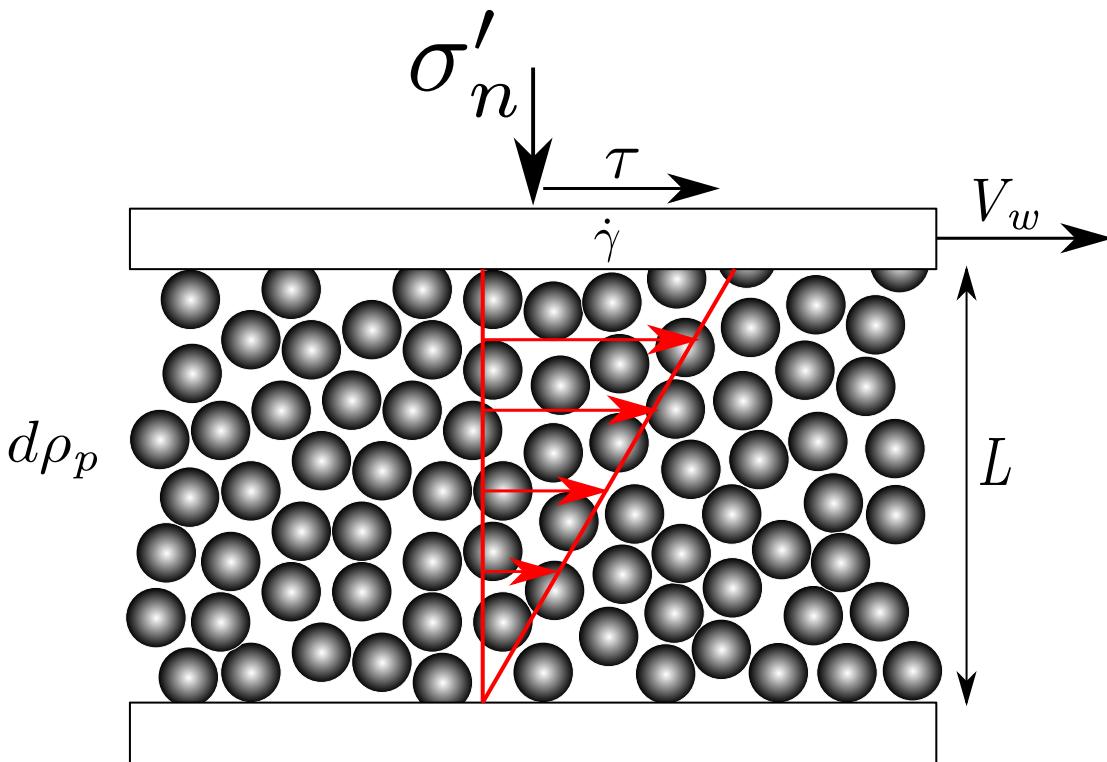


Figure 1.3 Plane shear stress distribution under a constant pressure and shear rate for a granular assembly

In general, the flow regimes can be classified based on the dimensionless number I (Da Cruz et al., 2005). Figure 1.5 shows the variation of frictional coefficient μ and packing fraction with dimensionless number I for different flow regimes under simple shearing. Dilute or “collisional” flow occurs for $I > 10^{-1}$ and the grain collision is chiefly binary, accompanied by additional “bounce-back” akin to gases (Kamrin, 2008). In the dilute flow regime, the grains are rarely in long-duration contacts and can be described by dissipative Boltzmann kinetics. The “quasi-static” regime occurs at the other extreme of the spectrum, $I < 10^{-3}$, where the intermittent motion is prevalent. The inertial time is always small enough for the grains to align to a dense compaction, without significant collisional dissipation. The frictional sliding and stick-slip dynamics dominate the dissipation mechanism. The

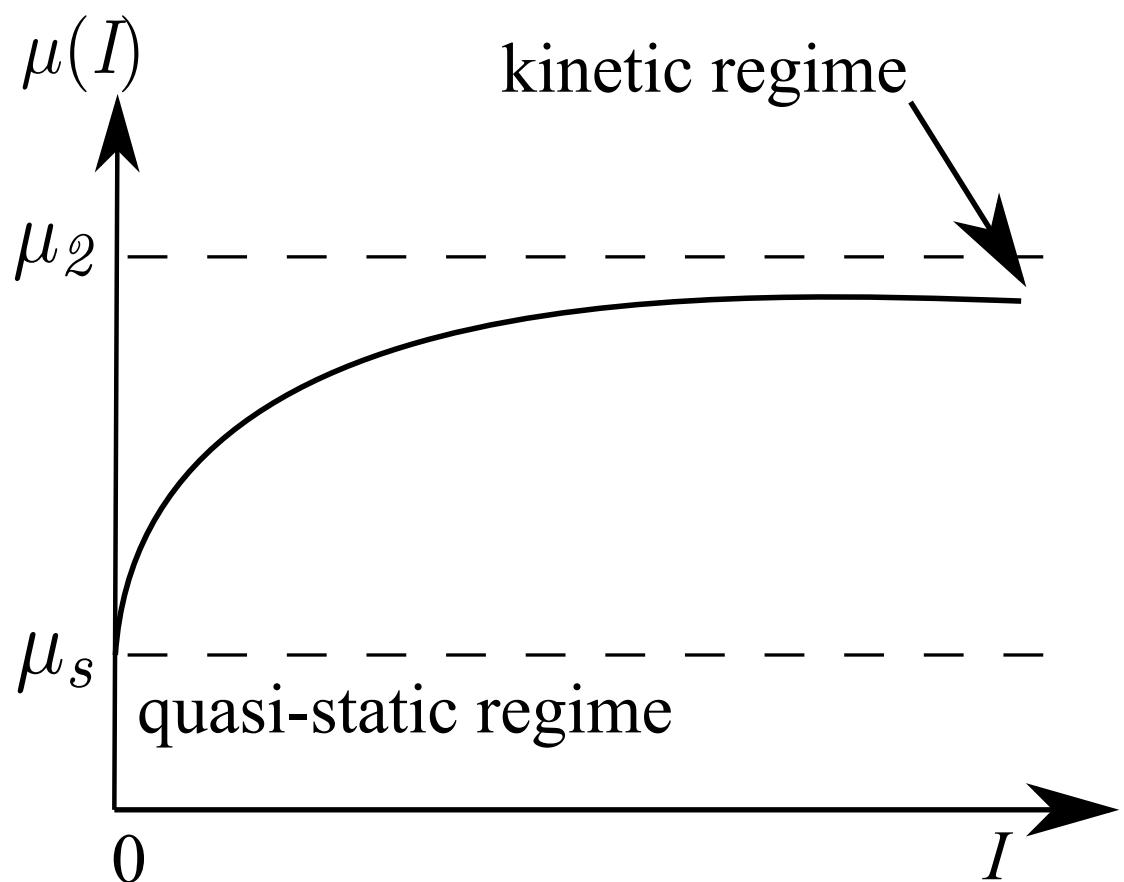


Figure 1.4 Sketch of dependence of frictional coefficient μ with dimensionless shear rate I , reproduced after Pouliquen et al. (2006)

stress/strain-rate relationship becomes singular; driving the system with a range of quasi-static normalized shear rates all give the same time-average value for μ . In this regime the dissipation is primarily frictional and rate-independent. The packing fraction appears to be independent of I , and grain-level interactions control to flow dynamics. The moderate-flow regime is observed for I between 10^{-3} and 10^{-1} , characterized by faster flows, with a high rate of contact formation and more energy dissipation per impact. In this regime, I has a one-one relationship with μ and is large enough for rate dependence, but small enough for the flow to remain dense. Moderate flows also exhibit the property of *shear rate dilation*, where an increase in the normalized flow rate causes the steady-state packing fraction to decrease, which is different from *shear dilation*, which refers to a decrease in the packing density as a function of total shear. Flows which are too slow to be moderate still undergo shear dilation due to geometric packing constraints, but shearing dilation occurs only in faster flows due to rate effects (Kamrin, 2008). In moderate flows, the dissipation is primarily rate-sensitive due to energy loss during contact formation, yet packing remains dense

Campbell (2002) described the “Moderate regime” as an elastic granular flow regime, where the inter-grain stiffness governs the overall flow behaviour of the granular assembly. At high concentration, the stresses are proportional to the contact stiffness, and the streaming stiffness, which reflect the momentum carried by the unsteady motions of particles as they move through the system, is negligible. When a dense granular assembly is sheared, the force chains that transmit the forces continue to rotate until they become unstable and collapse. As the force-chains rotate, the granular material tends to dilate. However it is restricted due to the constant volume constraint; instead, the rotation compresses the chain, generating an elastic response (Campbell, 2006). Campbell (2002) divided the flow into elastic and inertial regimes. In elastic regime, the force is transmitted principally through the deformation of force chains with a natural stress scaling of $\tau d/k_f$. The dimensionless parameter, k_f , is defined as the ratio of normal stiffness k_n to the applied normal pressure σ'_n . The force chains form when the grains are sheared at the rate of $\dot{\gamma}$, and hence the rate of chain formation is proportional to the shear rate $\dot{\gamma}$. This transitional regime can be explained using the force-chain concept. The lifetime of a force chain is proportional to $1/\dot{\gamma}$, consequently the product of rate of formation and the lifetime of the force chain is independent of $\dot{\gamma}$, and the stresses generated are quasi-static. However at higher shear rates, the elastic forces in the chain have to absorb the additional inertial force of the grains, requiring extra force to rotate the chain proportional to the shear rate. Even though the grains are locked in force chains, the forces generated must reflect the grain inertia. The ratio of elastic to inertial effects is

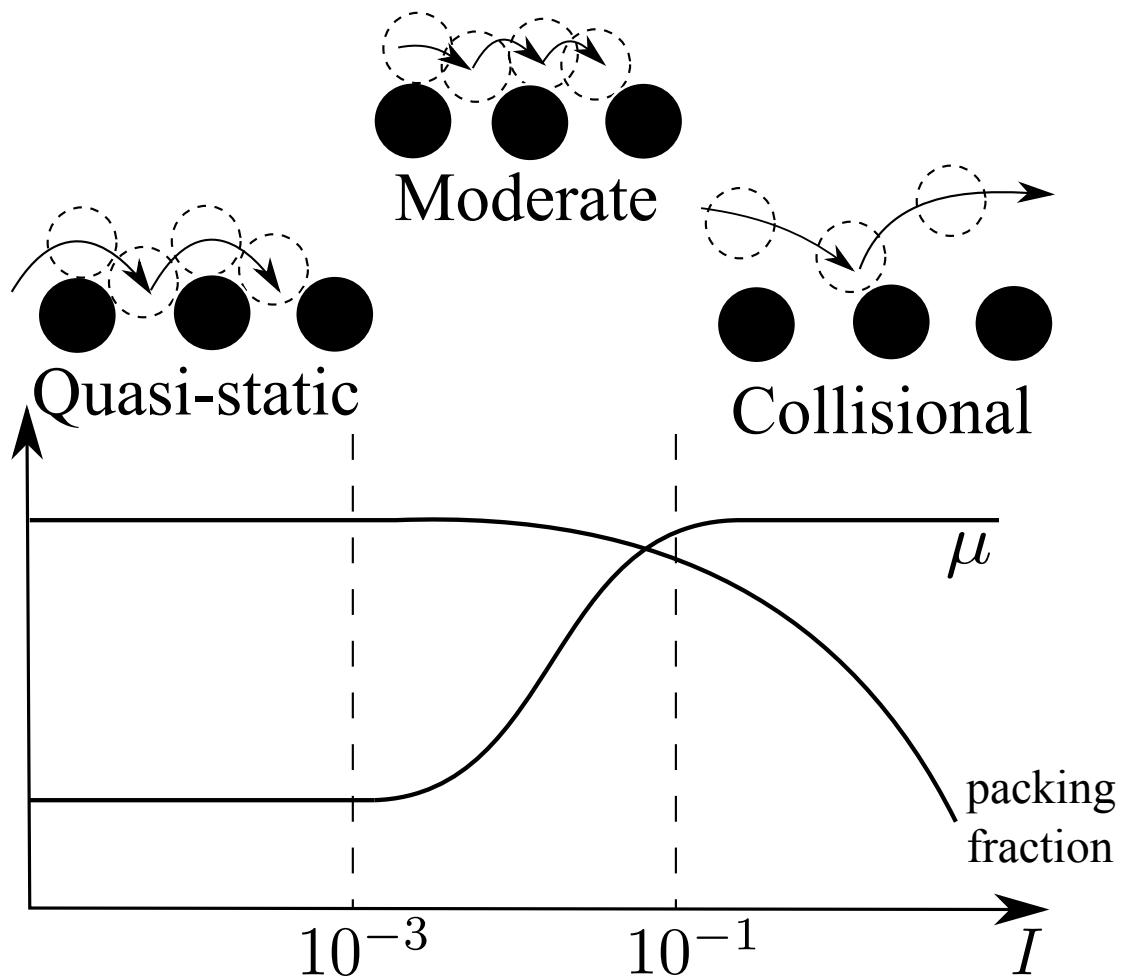


Figure 1.5 Variation of dimensionless parameter I for different flow regimes under simple shearing. (a) *Quasi-static* ($I < 10^{-3}$): Dissipation is primarily frictional and rate-independent. Packing fraction appears independent of I , and grain-level specifics are more important to flow dynamics; (b) *Moderate* ($10^{-3} < I < 10^{-1}$): the dissipation is primarily rate-sensitive due to energy loss during contact formation, yet packing remains dense; (c) *Collisional* ($I > 10^{-1}$): Flow becomes dilute and gas-like. Dynamics modelled best by dissipative Boltzmann kinetics. Redrawn after (Kamrin, 2008)

governed by a dimensionless parameter

$$k^* = \frac{k_f}{\rho d^3 \dot{\gamma}^2}, \quad (1.7)$$

where $k_f/\rho d^3 \dot{\gamma}^2 = (\tau/\rho d^2 \dot{\gamma}^2)/(\tau d/k_f)$ is the ratio of Bagnold's inertial to the elastic stress scaling. The important dimensionless parameter is k^* , which is a measure of inertially-induced deformation, reflects the relative effects of elastic to inertial forces, i.e. at large k^* , the elastic forces dominate and at small k^* , inertial forces dominate (Campbell, 2006).

Constitutive laws, which describe the dilatancy and friction, allow us to deduce the dependency of pressure and shear stress on shear rate and solid fraction. In contrast to the observation of Campbell (2002), Da Cruz et al. (2005) found that the normalised elastic stiffness k_f has little effect on the constitutive law, for values greater than 10^4 , however, it does affect the coordination number. Da Cruz et al. (2005) also observed that the microscopic friction coefficient, μ , has a significant influence on the dilatancy, and the solid fraction remains a linearly-decreasing function of I . The frictional properties of the material are found to control the solid fraction, from the critical state to the collisional regime (Da Cruz et al., 2005).

Although the rheology tends to describe the behaviour of granular flows, the mechanism of granular flows is found to vary with duration, position of granular material in the flow and pore-pressure feedback mechanism (Iverson, 2003). Rheology summarises the mechanical behaviour at scales that are smaller than the Representative Elemental Volume (REV), for a substance modelled as a continuum. Rheology-based descriptions are generally restricted to homogeneous materials that exhibit time-independent behaviour, hence are unsuitable for describing granular flows where the stress history has a significant effect on the flow dynamics. The estimation of debris flow yield strength highlights the limitation of rheologies which do not consider the development of strength with evolution of time and space. Johnson (1965) emphasized that debris yield strength is predominantly a frictional phenomenon analogous to the Coulomb strength of granular soils, and that strength consequently varies with effective normal stress. Treatment of yield strength as an adjustable rheological property contradicts the basic understanding that the strength evolves as the debris-flow motion progresses. Frictional behaviour implies no explicit dependence of shear resistance on shear rate, whereas rheological formulas commonly used to model debris flows generally include a viscous component that specifies a fixed functional relationship between shear resistances and shear rate. Although rate-dependent shear resistance is observed in debris flows, its magnitude and origin indicate that it is ancillary rather than essential (Iverson, 2003).

1.2.4 Shallow-water approximation

Developing constitutive laws valid from the quasi-static to dilute regimes remains a serious challenge. Simple elasto-plastic approach fails to model the collisional regimes in a granular flow. On the other hand, the original kinetic theory based on binary collisions does not capture the correct behaviour in the dense regime. In configurations where the flowing layer is thin, a different theoretical framework is adopted. One such approach is the depth-averaged shallow-water equation, which has been applied to solve granular flow dynamics with a reasonable amount of success. The Savage-Hutter model (Savage and Hutter, 1991), is a depth-average continuum-mechanics based approach which consists of hyperbolic partial differential equations to describe the distribution of the depth and the topography of an avalanching mass of cohesion-less granular media (Hutter et al., 2005). This approach is based on the assumption that the horizontal length scale is very large in comparison with the vertical length scale, which allows us to neglect the horizontal partial derivatives relative to the vertical partial derivatives. Field observations of natural avalanches indicate an aspect ratio of 10^{-3} to 10^{-4} (Cawthor, 2006). By neglecting the vertical length scale, the continuum equation for conservation of mass and momentum can be written as

$$\partial_x u + \partial_y v = 0, \quad (1.8)$$

$$\partial_t u + u \partial_x u + v \partial_y u = (\nabla \cdot \boldsymbol{\sigma})_x + \mathbf{F}_x. \quad (1.9)$$

The continuum equation requires determining the components of the stress tensor and a suitable constitutive law. *Savage-Hutter (SH) model* uses the Mohr-Coulomb law to describe the constitutive relation. The conservation of mass and momentum in the SH model is based on the assumption of granular flow as an incompressible fluid flow, which means that throughout the avalanche, the density of the avalanching material remains constant. Although Hutter et al. (1995) observed the density of the granular flow to remain almost constant in a flow down a curved chute, the destructive nature of landslides and avalanches restricts us from inferring a conclusive result. The SH model involves the following assumptions: (1) Coulomb-type sliding takes place with a bed friction angle δ , (2) Mohr-Coulomb frictional behaviour occurs inside the material with internal angle of friction, $\phi \geq \delta$, and (3) the velocity profile is assumed to be uniform throughout the avalanche depth. The granular flow over a rigid plane inclined at an angle, θ is shown in figure 1.6. The mass and momentum balance in the SH model is written as

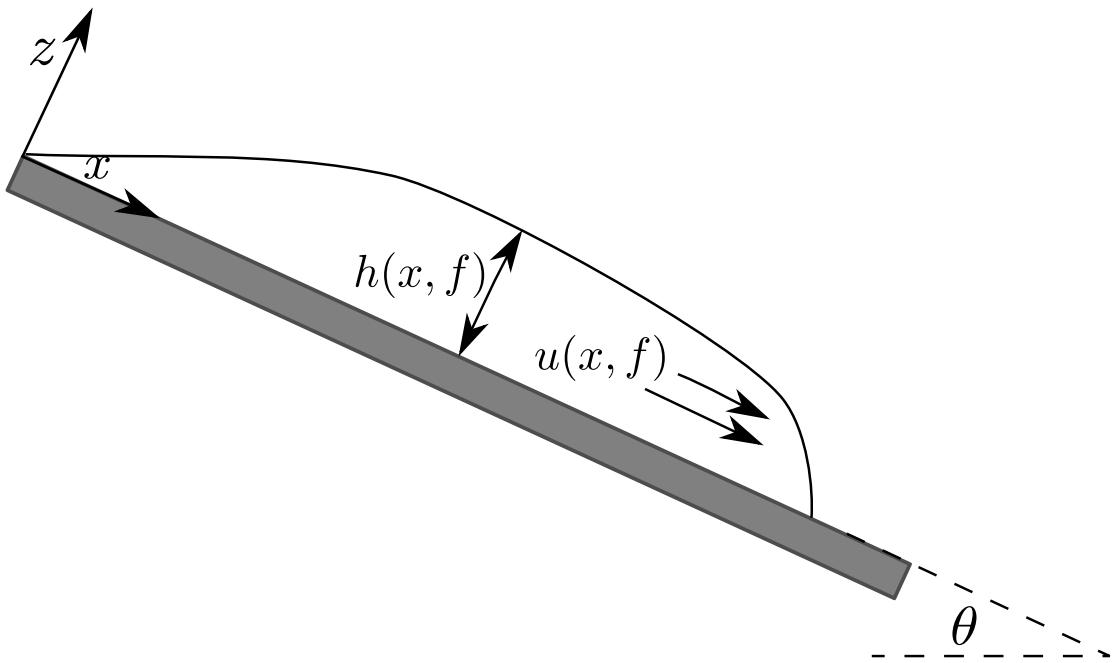


Figure 1.6 Illustration of the Savage-Hutter model

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(hu) = 0, \quad (1.10)$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = (\sin \theta - \tan \delta \operatorname{sgn}(u) \cos \theta) - \beta \frac{\partial h}{\partial x}, \quad (1.11)$$

where capital letters denote non-dimensional quantities with respect to the typical horizontal and vertical length scales (l^*, h^*) and the time scale $\sqrt{l^*/g}$. The key feature in the shallow water approximation is the Mohr-Coulomb constitutive law, which is applied at the free surface and at the base, to describe the granular flow. Comparison of the model with the post-calculation of Madlein avalanche in Austria indicates that the Coulomb basal friction is insufficient and requires an additional viscous component. The SH model's predictions were not satisfactory for granular flows down gentle slopes of inclination angle $\leq 30^\circ$, where granular materials exhibit premature stop (Hutter et al., 2005). The SH model has not yet been tested in cases where the granular flow interacts with obstacles.

The two main modelling techniques that are commonly employed to describe granular flow are the continuum approach and the discrete element approach. The continuum approach involves treating granular assembly as a continuum and describing its response using constitutive laws, while the discrete approach involves considering the individual grains of the granular material and applying Newton's laws of motion to describe the deformation of the granular material. These approaches are adopted in the present study and detailed discussions are provided in chapter 2.

1.3 Studies on granular flows

The flow of dense granular material is a common phenomenon in engineering predictions, such as avalanche, landslides, and debris-flow modelling. Despite the huge amount of research that has gone into describing the behaviour of granular flow, a constitutive equation that describes the overall behaviour of a flowing granular material is still lacking. To model geo-physical scale problems, the depth-averaged constitutive equations have been employed along with an empirical friction coefficient and a velocity profile deduced from experiments (Iverson, 2003; Midi, 2004; Pouliquen, 1999). Although this approach has been successful to a certain extent in predicting geophysical flows (Hutter et al., 1995; Pouliquen and Chevoir, 2002), it presents two important shortcomings (Lajeunesse et al., 2005): first, the depth-average method is true only if the thickness of the flowing layer is thin in comparison with the lateral dimension, and second, the empirical laws are deduced from experiments performed under steady-flow conditions. These cast doubts on the validity of the depth-averaged approach. Two simple granular flow studies, granular column collapse and granular flow down an inclined plane, carried out by various researchers to understand the flow behaviour are discussed below.

1.3.1 Granular column collapse

Lube et al. (2005) and Lajeunesse et al. (2004) have carried out experimental investigations on the collapse behaviour of granular columns on a horizontal plane. Both the experiments involved filling a column of height H_0 and length L_0 with granular material of mass m . Figure 1.7 shows the schematic view of the experimental configuration of a quasi-two-dimensional granular column collapse in a rectangular channel. The granular column is then released *en masse* by quickly removing the gate, thus allowing the granular material to collapse onto the horizontal surface, forming a deposit having a final height H_f and radius L_f . Although the experiment is simple and attractive allowing us to explore the limitations of depth-average modelling techniques, a constitutive law that could describe the entire flow behaviour is still lacking. The primary aim of these experiments was to determine the scaling laws for the run-out distance.

Deposit morphology

Experimental findings

Lajeunesse et al. (2005) observed that the flow dynamics and the final run-out distance remain independent of the volume of granular material that is released, but depend only on

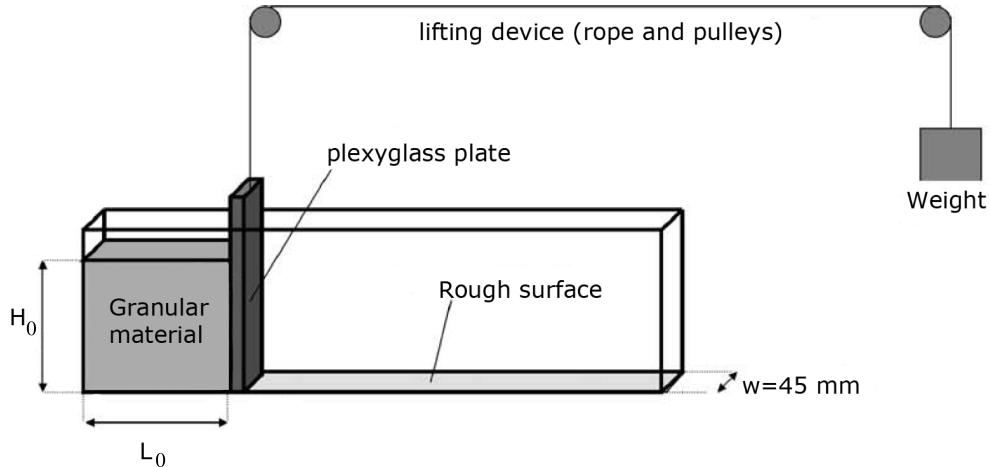


Figure 1.7 Schematic view of the experimental configuration of a quasi-two-dimensional granular column collapse in a rectangular channel (Lajeunesse et al., 2004)

the initial aspect ratio a of the granular column. The experiment was carried out to understand the effect of the geometrical configuration on the run-out, the mechanism of initiation of the flow, the evolution of flow with time, and to understand how such complex flow dynamics could produce deposits obeying simple power laws. Lube et al. (2005) explored the effect of density and shape of grains on flow dynamics, whereas Lajeunesse et al. (2004) worked with glass beads to study the influence of bead size and substrate properties on the deposit morphology. Surprisingly, both drew the striking conclusion that the flow duration, the spreading velocity, the final extent of the deposit, and the fraction of energy dissipated during the flow can be scaled in a quantitative way independent of substrate properties, bead size, density, and shape of the granular material and released mass, m (Lajeunesse et al., 2005).

The normalised final run-out distance as a function of the initial aspect ratios of the granular column under plane-strain and axisymmetric conditions is shown in figure 1.8a. Lube et al. (2005) scaled the run-out distance as

$$\frac{L_f - L_0}{L_0} \approx \begin{cases} 1.24a, & a \lesssim 1.7 \\ 1.6a^{1.2}, & a \gtrsim 1.7 \end{cases} \quad (1.12)$$

while Lajeunesse et al. (2005) scaled the run-out distance as

$$\frac{L_f - L_0}{L_0} \approx \begin{cases} 1.35a, & a \lesssim 0.74 \\ 2.0a^{1.2}, & a \gtrsim 0.74 \end{cases} \quad (1.13)$$

The final run-out distance is found to have a linear relationship for short columns and exhibit a power-law relation with the initial aspect ratio of tall columns.

The normalised final height as a function of the initial aspect ratios of the granular column under plane-strain and axisymmetric conditions is shown in figure 1.8b. The evolution of the final scaled deposit height H_f/L_0 with the initial aspect ratio a for the axisymmetric collapse (Lajeunesse et al., 2005) is given as

$$H_f/L_0 \approx \begin{cases} a, & a \lesssim 0.74 \\ 0.74, & a \gtrsim 0.74 \end{cases} \quad (1.14)$$

and for two-dimensional collapse

$$H_f/L_0 \approx \begin{cases} a, & a \lesssim 0.7 \\ a^{1/3}, & a \gtrsim 0.7 \end{cases} \quad (1.15)$$

The final height of collapse is unaffected in both 2D collapse and axisymmetric collapse for short columns. In the case of tall columns, axisymmetric collapse show a constant final height whereas a power-law relation with the initial aspect ratio is observed in 2D collapse.

Axisymmetric versus two-dimensional collapse

Quasi-two-dimensional collapse of a granular column on a horizontal surface reveals that the geometric configuration influences the scaling of the run-out distance (Lajeunesse et al., 2005). The run-out in a quasi-two-dimensional collapse of a granular column in a rectangular channel scales as

$$\frac{L_f - L_0}{L_0} \approx \begin{cases} 1.2a, & a \lesssim 2.3 \\ 1.9a^{2/3}, & a \gtrsim 2.3 \end{cases} \quad (1.16)$$

Balmforth and Kerswell (2005) studied the collapse of granular columns in rectangular channels with a narrow (width W of the slot = 10 * diameter d) and a wide slot ($W = 200 * d$), and focused on the deposit shape. Lacaze et al. (2008) observed that slots with width $W \geq 1.2 \times d$ do not crystallise and wider slots $W \geq 2 \times d$ overcomes the effect of jamming. As in the axisymmetric case, Balmforth and Kerswell (2005) observed that the run-out is well represented at large aspect ratios by a simple power-law expression, which depends on the width of the channel. The run-out distance can be scaled as: $\Delta L/L_0 \approx \lambda a^{0.65}$ for narrow channels and $\Delta L/L_0 \approx \lambda a^{0.9}$ for wide channels. The scaling found for quasi-two-dimensional experiments in the narrow gap configuration gives similar results to those

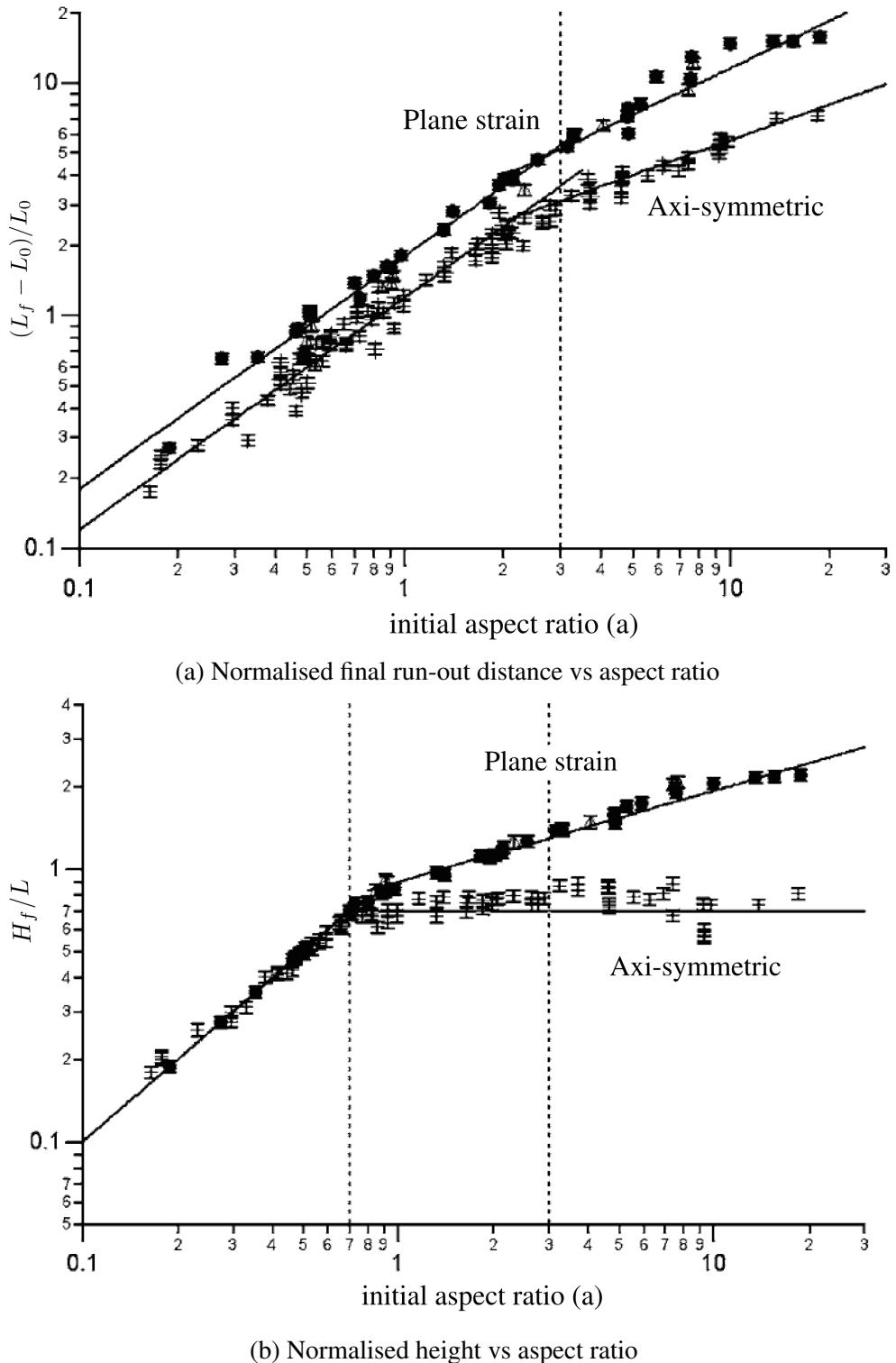


Figure 1.8 The normalised final run-out distance and final height as a function of the initial aspect ratios of the granular column under plane-strain and axisymmetric conditions (Lajeunesse et al., 2004).

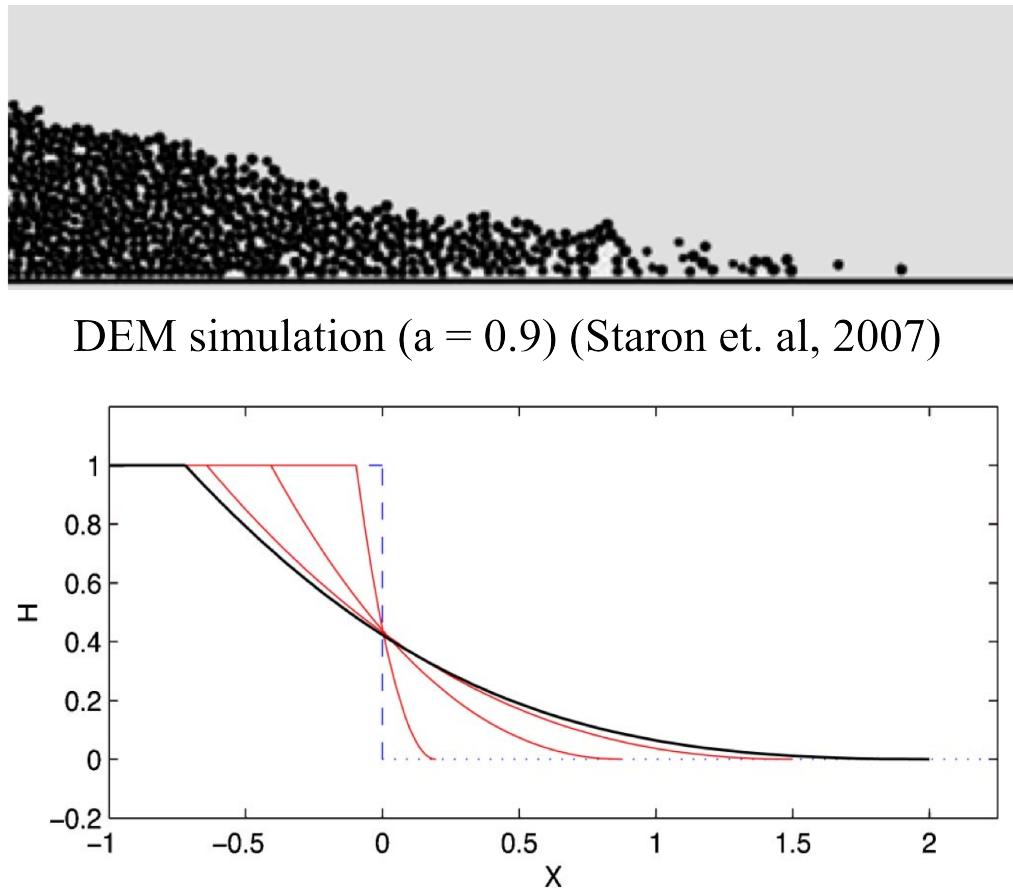
reported by Lube et al. (2005) and roughly a scaling of $(L_f - L_0)/L_0 \propto a^{2/3}$. However, these laws are influenced by the presence of sidewalls and depend, albeit only in the numerical coefficient of proportionality, on the frictional properties of the granular material.

Balmforth and Kerswell (2005) observed that the constant of proportionality λ in the power-law relation is found to vary with the internal friction angle of the granular material, which contradicts the findings of previous authors, especially Lube et al. (2005) who found that the scaling of run-out is independent of the granular material. This may perhaps be due to a narrow range of experimental materials and grain size distributions considered in the previous studies. Balmforth and Kerswell (2005) found that the material properties have almost no influence on the exponent of the normalised run-out as a function of the initial aspect ratio. The numerical constant of proportionality, however, showed clear material dependence. This corroborates the conclusions of Lajeunesse et al. (2004). Daerr and Douady (1999) also observed strong influence of initial packing density and the internal structure on the behaviour of granular flows. By comparing the initial and final cross-section areas of the pile, Balmforth and Kerswell (2005) observed that the granular material experienced dilation (by about 10%) as the flow progressed to form the final deposit (Balmforth and Kerswell, 2005). Although, internal packing structure and density is found to have an influence on the run-out behaviour, a proper understanding of the effect of density on the run-out and evolution of packing fraction is still lacking.

Numerical modelling

Numerical simulations of granular column collapse by Zenit (2005) and Staron and Hinch (2007) yielded similar scaling of run-out with aspect ratio a . Unlike other authors, Zenit (2005) did not observe any transition in the run-out behaviour of a granular column collapse with the aspect ratio a . The origin of the exponents is still under discussion. No model has yet achieved a comprehensive explanation of the complex-collapse dynamics. For higher aspect ratios, the free fall of the column controls the dynamics of the collapse and the energy dissipation at the base is attributed to the coefficient of restitution. Thus, the initial potential energy stored in the system is dissipated by sideways flow of material and the mass ejected sideways is found to play a significant role in the spreading process, i.e. as a increases, the same fraction of initial potential energy drives an increasing proportion of initial mass against friction, thus explaining the power-law dependence of the run-out distance on a .

Taking advantage of the similarity between granular slumping and the classical “*dam break*” problem in fluid mechanics, Kerswell (2005) solved both the axisymmetric and two-dimensional granular-collapse problem using the shallow-water approximation. Although the results of the shallow-water approximation have good agreement with experimental



Shallow water approximation ($a = 1.0$) (Kerswell, 2005)

Figure 1.9 Collapse of granular column simulation using DEM (Staron and Hinch, 2007) and Shallow-water approximation (Kerswell, 2005).

results, the shallow-water approximation overestimates the run-out distance for columns with aspect ratio a greater than unity. The shallow-water equation does not take into account the effect of vertical acceleration (Lajeunesse et al., 2005), which has been found to play a significant role in controlling the collapse dynamics (Staron and Hinch, 2007), thus resulting in overestimation of the run-out distance. The evolution of run-out predicted using shallow-water approximation and DEM are shown in figure 1.9. Tall columns showed significantly longer run-out distances when using continuum approaches like the material point method (Bandara, 2013; Mast et al., 2014a). It was observed that a simple friction model cannot effectively describe the collapse dynamics (Staron and Hinch, 2007). However, the reason for difference in the run-out behaviour is not known.

The final collapse height observed in the numerical simulations of granular collapse is found to be similar to the experimental results (Balmforth and Kerswell, 2005; Lube et al., 2005). Numerical simulation of granular column collapse (Lacaze et al., 2008; Staron and Hinch, 2007) showed a transition in the flow behaviour at $a \geq 10$, which was not observed in granular collapse experiments (Balmforth and Kerswell, 2005; Lajeunesse et al., 2004; Lube et al., 2005). In the depth-averaged shallow-water model, which integrates over the depth, the emphasis was on capturing the scaling of the final deposit, rather than trying to reproduce the internal structure of the flow. The shallow-water model captures well the final deposit scaling for lower aspect ratios, however fails to capture the flow dynamics for granular columns with higher aspect ratios, where the flow is governed mainly by the vertical collapse of the granular column as a whole. The run-out distance predicted is clearly erroneous in the collapse regime where there is a sudden drop in efficiency by which the initial potential energy of the system is converted into the kinetic energy for spreading. Even a more sophisticated basal drag law will not be sufficient to model the mechanism of granular column collapse realistically using the shallow-water approximation (Kerswell, 2005). Considering the large spectrum of theoretical frameworks, no consensus exist on the origin of the power-law and finding constitutive laws valid from the quasi-static to dilute regimes remains a serious challenge.

Flow dynamics

Experimental findings

The final scaled run-out distance shows a transition from a linear to a power-law relationship with the initial aspect ratio of the column at an aspect ratio of 1.7, indicating a transformation in the spreading process or the collapse mechanism. To understand the collapse mechanism, it is insufficient to study only the final scaled profile, and hence the entire flow process should be analysed. Lajeunesse et al. (2005) observed the flow regime and deposit morphology for a quasi-two-dimensional granular collapse in a rectangular channel. The flow phenomenology of a granular column collapse in a rectangular channel was surprisingly similar to that observed in the axisymmetric collapse (Lajeunesse et al., 2004; Lube et al., 2005), depending mainly on the initial aspect ratio a (section 1.3.1).

The flow dynamics involves spreading of granular mass by avalanching of flanks producing a truncated cone for $a \lesssim 0.74$ and a cone for $a \gtrsim 0.74$; the transition of flow dynamics occurs as the value of a is increased (figure 1.10). The evolution of the deposit height remains independent of the flow for $a \lesssim 0.7$, however it exhibits significant dependence on the geometrical configuration for $a \gtrsim 0.7$. In rectangular channels, the effect of side-wall on the run-out behaviour was observed; the surface velocity profile between the side walls

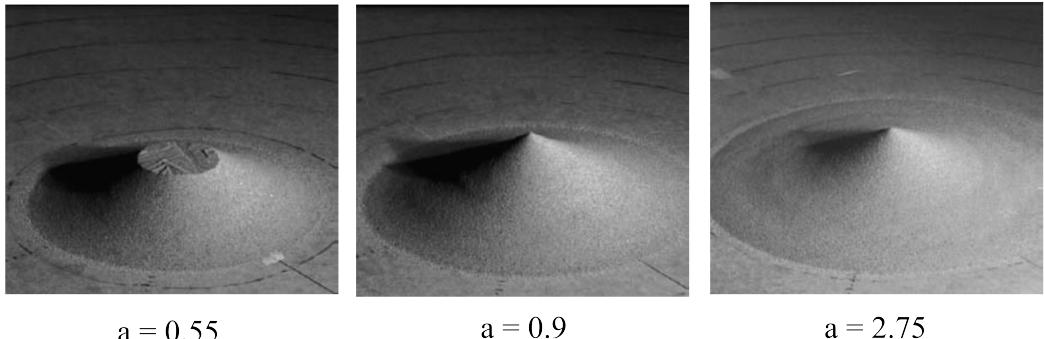


Figure 1.10 Final deposit profiles for granular column collapse experiments with different initial aspect ratios (Lube et al., 2005).

is that of a plug flow with a high slip velocity at the wall and low shear along the direction transverse to the flow. Systematic measurements indicate that the ratio of the maximum surface velocity to the surface velocity at the wall is between 1.2 and 1.4. Lajeunesse et al. (2005) observed that the difference between the evolution of H_f in the axisymmetric geometry and in the rectangular channel is not an experimental artefact due to the side wall friction, but is a *geometrical effect*.

Understanding the internal flow structure will provide an insight into the complex collapse dynamics. The failure surface observed at $t = 0.4\tau_c$, where τ_c is the critical time at which the flow is fully mobilised, for granular columns with initial aspect ratio of 0.4 and 3 are shown in figure 1.11. For smaller values of aspect ratio $a \leq 0.7$, the flow is initiated by a failure at the edge of the pile along a well-defined shear band above which material slides down and below which the grains remain static. The grains located above the shear-failure surface move “*en masse*” and most of the shear is concentrated along this surface forming a “*truncated-cone-like*” deposit with a central motionless plateau figure 1.11. For columns with larger aspect ratios, the flow is still initiated by failure along a well-defined surface, an inclined plane in two-dimensional geometry or a cone in the axisymmetric case. However, the initial height of the column is much higher than the top of the failure surface, causing a vertical fall of grains until they reach the summit where they diverge along the horizontal direction, dissipating a lot of kinetic energy, resulting in a final conical deposit. Interestingly, the final deposit height coincides with the summit of the failure surface in the axisymmetric geometry, whereas in the rectangular channel, the deposit summit always lies above the top of the failure surface (Lajeunesse et al., 2005). Shallow-water approximations show a truncated cone-like deposit, while DEM simulations show a cone like deposit for $a = 1.0$ (figure 1.9). This shows the inability of the shallow-water approximation to model tall columns.

Identification of the static region is an important task, as it is a prime component in describing the collapse mechanism. Regardless of the experimental configuration, for all

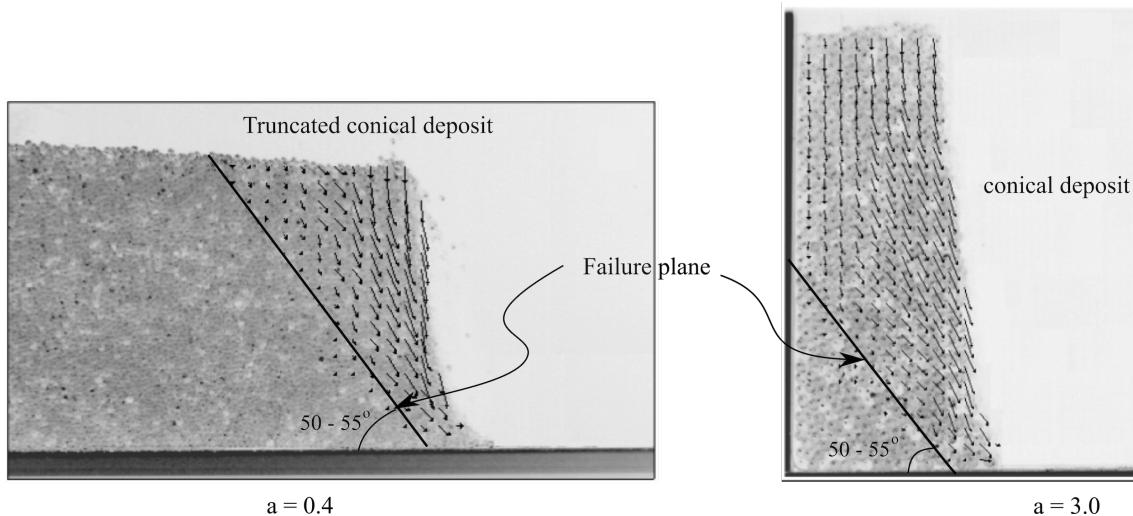


Figure 1.11 The extent of the failure surface for granular columns with initial aspect ratio of 0.4 and 3 at time $t = 0.4\tau_c$ (Lajeunesse et al., 2004). Short columns show truncated conical deposit at the end of the flow, while tall columns exhibit conical deposit.

values of a the flow is initiated by rupture along a well-defined failure surface and the failure angle remains of the order of 50° to 55° (figure 1.11). The failure angle is consistent with an interpretation of *active Coulomb failure*, which leads to a failure angle $\phi_f = 45^\circ + \phi'/2$, where ϕ' is the internal friction angle of the granular material. Estimating the internal friction angle of glass beads from the angle of repose as 22° , the failure angle is estimated as 56° , which is in good agreement with the experimental findings. Contrary to the suggestion of Lajeunesse et al. (2004), the shear-failure angle was found to have no direct effect on the transition between truncated cone and conical deposit occurring at aspect ratio a of 0.7 (Lajeunesse et al., 2005). Schaefer (1990) observed the onset of instability in a narrow wedge of 56° to 65° , which corresponds to the angle of shear bands. A rate-dependent constitutive relationship (Jop et al., 2006) for dense granular flows indicates the angle of shear-band orientation depends on the inertial number I . For small to moderate values of I , the orientation of shear bands is found to vary from the Roscoe and the Coulomb solutions to a unique admissible angle (Lemiale et al., 2011). Daerr and Douady (1999) observed active Coulomb-type yielding in transient surface flows for granular materials having a packing density of 0.62 to 0.65.

Numerical findings

In order to describe the complex flow dynamics, it is important to understand the internal structure and the flow behaviour. The flow evolution involves three stages (Staron and Hinch, 2007). The first stage involves conversion of the initial potential energy of the grains into

vertical motion, resulting in downwards acceleration of grains. In the second stage, the grains undergo collision with the base and/or neighbouring grains, and their vertical motion is converted into horizontal motion. The velocity field depends on the position of grains along the pile. In the region above the static core, the flow is locally parallel to the failure surface and has an upper linear part and a lower exponential tail near the static bed (figure 1.11). The velocity flow profile is similar to that of a steady granular flow (Midi, 2004). In the final stage, the grains eventually leave the base area of the column and flow sideways. At the front, the flow involves the entire thickness of the pile and corresponds to a plug flow in the horizontal direction. The typical velocity observed at the front of the ejecting mass is $v = \sqrt{2gL_0}$. As the pile spreads, interface separation occurs as the flow diverges and the static region starts to move inwards; this effect is predominant in the case of granular flows in a rectangular channel.

The typical time required for the flow to cease and form the final deposit, from the instant of its release, is $\tau_c = \sqrt{H_0/g}$ (Staron and Hinch, 2007). While plotting the variation of normalized potential and kinetic energy with normalized time, Staron and Hinch (2007) observed that the flow ceases when the normalized time t/τ_c is 2.5, i.e. the flow is assumed to have stopped when the total normalized energy is almost zero. This observation is consistent with the experimental results of Lube et al. (2005) and Lajeunesse et al. (2005). The transition of the flow occurs when the normalized time t/τ_c is 1.0, which is defined as the critical time at which the flow is fully mobilized.

Comments on modelling

In order to have a detailed understanding of the final profile of the collapsed granular column, it is important to solve the collapse problem as an *initial-value problem* (Balmforth and Kerswell, 2005), beginning from the instant of release and extending to the time when the material finally ceases to flow, forming the final deposit. As the process of granular collapse involves collective dynamics of collisions and momentum transfer, the prediction of the trajectory of a single grain is difficult. In fact, there are quantitative disagreements between theory and experiments; the final shapes are reproducible, but not perfectly. Some of the disagreement arises because the experiments did not have exactly the same amount of materials; it is indeed difficult to fill the pile with exactly the same amount of material, which results in differences in packing. However, the theoretical errors are due to the incapability of the models to capture the physics that governs the flow dynamics (Balmforth and Kerswell, 2005).

Shallow water models fail to account for the vertical acceleration, which is responsible for the momentum transfer and, in turn, the spreading process. This restricts the shallow

water model to capture the mechanism of collapse until the critical time τ_c . Surprisingly, shallow-water models capture certain experimental aspects for columns with lower aspect ratios (Balmforth and Kerswell, 2005; Kerswell, 2005; Mangeney et al., 2010), even though the contrast between surface flows and the static region is important in this range of aspect ratio. Thus, the assumption of plug flow in the horizontal direction is not critical in capturing the run-out behaviour, especially if the basal friction coefficient is used as a fitting parameter (Lajeunesse et al., 2005).

Simple mathematical models based on conservation of horizontal momentum capture the scaling laws of the final deposit, however they fail to describe the initial transition regime, indicating that the initial transition has negligible effect on the run-out, which is incorrect. Models based on the initial potential energy show promise, but the effect of material properties, such as basal friction and coefficient of restitution, on the run-out behaviour is still unclear and produces non-physical run-outs. The $\mu(I)$ rheology predicts the normalized run-out behaviour quite well in comparison with the experimental results, for lower aspect ratios. The spreading dynamics is found to be similar for the continuum and grain approaches; however, the rheology falls short in predicting the run-out distance for higher aspect ratios.

Unlike Lube et al. (2005), many researchers (Balmforth and Kerswell, 2005; Kerswell, 2005) observed strong dependency of material properties on the run-out distance, moistening the materials or the sides of the channel even by a small amount leads to markedly different results. Staron and Hinch (2007) observed that the friction has little effect on the run-out for granular column collapse for high aspect ratios, which are driven mainly by the free vertical fall of grains. The initial conditions have a significant impact on the overall behaviour of the granular system, indicating the significance of the triggering mechanism in case of the natural flows (Staron and Hinch, 2007). A theoretical framework that is capable of describing the influence of material properties on the run-out behaviour is still lacking. Numerical investigations, such as Discrete Element Method techniques, allow us to evaluate these quantities which are not accessible experimentally, thus providing useful insight into the flow dynamics. Subsequent chapters discuss the methodology and modelling of granular column by continuum- and discrete-element approaches. Effect of initial packing fraction and the internal structure on the run-out behaviour are also discussed. The difference in the mechanism of modelling the granular flows in continuum and discrete approaches are presented in ??.

1.3.2 Flow down an inclined plane

Most contemporary research on granular materials deals with steady-state flow. Transients and inhomogeneous boundary conditions are much less amenable to observation and analysis,

and have thus been less extensively studied despite their primary importance in engineering practice. Studies on the flow of granular materials down inclined planes are important to understand the mechanism of geophysical hazards, such as granular avalanches, debris flows and submarine landslides. Large scale field tests on dry and saturated granular materials were carried out to capture the mechanism of granular flows down an inclined plane (Denlinger and Iverson, 2001; Okada and Ochiai, 2008).

Experimental findings

Granular material stored in a reservoir at the top of the inclined plane is released by opening a gate (figure 1.12). The flow rate is controlled by the height of the opening. The material flows down and develops into a dense granular flow. An initially static granular layer of uniform thickness ' h ' starts to flow when the plane inclination reaches a critical angle, θ_{start} , the material reaches a sustained flow until the inclination is decreased down to a second critical angle, θ_{stop} (Midi, 2004). The occurrence of two critical angles indicates the hysteretic nature of granular materials. Reciprocally, the critical angle thresholds can be interpreted in terms of critical layer thickness $h_{stop}(\theta)$ and $h_{start}(\theta)$. The measurement of $h_{stop}(\phi)$ is easier as it corresponds to the thickness of the deposit remaining on the plane once the flow has ceased.

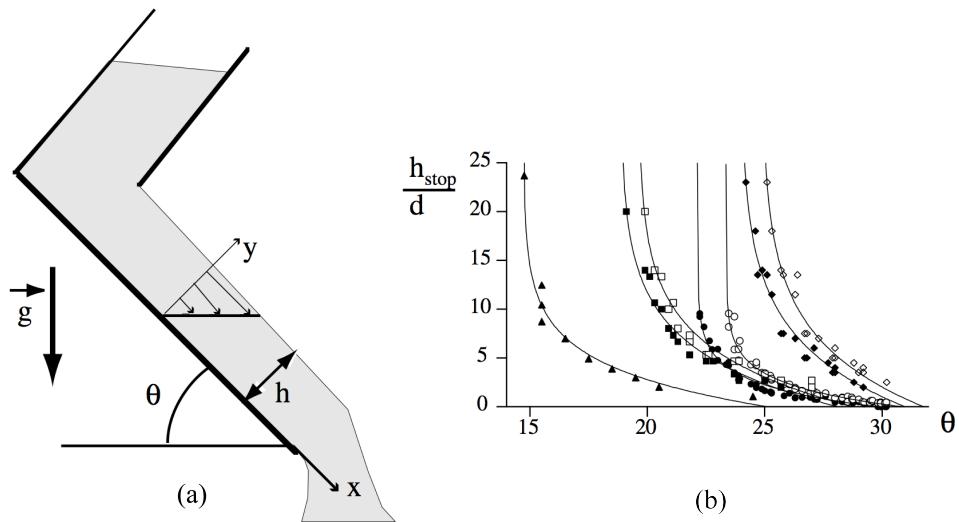


Figure 1.12 Rough inclined plane: (a) Set-up, and (b) $h_{stop}(\theta)$ (black symbols) and $h_{start}(\theta)$ (white symbols). Reproduced after (Midi, 2004).

The two curves $h_{stop}(\theta)$ and $h_{start}(\theta)$ divide the phase diagram (h, θ) into three regions: a region where no flow occurs, ($h < h_{stop}(\theta)$), a sub-critical region where both static and flowing layers can exist ($h_{stop}(\theta) < h < h_{start}(\theta)$) and a region where flow always occurs,

$(h > h_{start}(\theta))$. In the flow regime, i.e. $(h > h_{start}(\theta))$, the flow is steady and uniform for moderate inclination, but accelerates along the plane for large inclinations (Midi, 2004). The critical angle controlling the flow behaviour tends to increase when the thickness of the bed decreases (Daerr and Douady, 1999; Pouliquen and Chevoir, 2002), which can be attributed to non-trivial finite-size effects and/or boundary effects that are not well understood (Forterre and Pouliquen, 2008). There exists a value of roughness for which a maximum thickness of deposit is observed, which might correspond to a maximum of effective friction at the bottom (Midi, 2004).

For thick enough piles flowing on a rough inclined plane, say $h \geq 20 \times d$, the velocity profiles and rheology follow Bagnold scaling. As the height of the flowing pile reduces, a continuous transition from Bagnold rheology to linear velocity profiles through to avalanche-like dynamics occurs, until finally, one reaches the angle of repose θ_r , and the flow ceases. This transition behaviour is difficult to model.

Numerical modelling

Fast moving granular flows can undergo a motion-induced self-fluidisation process under the combined effects of flow front instabilities setting on at large values of the Froude number which are responsible for extensive entrainment, and longer time between collisions of soil grains. Self-fluidisation results in enhanced mobility of the solids, causing an inviscid flow (Bareschino et al., 2008). It is understood that, for a granular material to flow, it has to exceed a certain critical threshold, i.e. the friction criterion: the ratio of shear stress to normal stress. As there is no internal stress scale for a granular material, granular materials exhibit solid-fluid transition behaviour based on the friction criterion (Forterre and Pouliquen, 2008). The stress ratio in the flowing regime above the static bed indicates that the solid-to-fluid transition is a yielding phenomenon and can be described by Mohr-Coulomb-like failure criterion (Zhang and Campbell, 1992). This is in contrast to the mechanism of behaviour of other complex fluids, where there is an internal stress scale linked to the breakage of microscopic structure. From a microscopic point of view, the strength of granular materials is due to the internal friction between grains, but packed frictionless materials still exhibit macroscopic friction.

Constitutive laws based on plasticity theories relate the micro-structure to the macroscopic behaviour (Roux and Combe, 2002), which provide useful insight into the mechanism of granular flow. However, at present they are limited to initiation of deformation and do not predict quasi-static flow. Continuum approaches such as the Material Point Method simulation of granular flow down an inclined plane (Abe et al., 2006; Bandara, 2013) capture the flow behaviour in the initial stages, however the model exhibits inconsistent behaviour

when the granular material ceases to flow. This may be due to the application of small deformation theory to a large deformation problem and the use of zero dilation.

Alternatively by using the $\mu(I)$ rheology we can capture the velocity profile and the localization at the free surface. However, it fails to model the transition from a continuous flow to an avalanching regime as the flow rate is decreased (Pouliquen et al., 2006). The rheology predicts no-flow below a critical angle $\theta_s = \arctan(\mu_s)$ independent of the thickness. In experiments, it is observed that the critical angle increases when the thickness of the flow decreases (Pouliquen, 1999). Granular flow down rough inclined planes exhibits strong Coulomb shear stresses on a plane normal to the basal flow boundary. The stresses dissipate the energy along the rough surface; models that lack multi-dimensional momentum transport or Coulomb friction cannot represent this energy dissipation.

Comments on modelling

Granular flow down inclined planes exhibits a transient behaviour. Various velocity profiles and flow behaviours can be obtained not only through changing the height of the flowing granular mass, but also by varying the inclination of the chute, such that there is an overlap region where one can obtain similar flow properties through either procedure. These features can be used to better predict the evolution of an avalanche surface. The experimental configuration is ideal to study the effectiveness of various theoretical frameworks in modelling granular flows, especially the transition from solid-like to fluid-like behaviour. The $\mu(I)$ rheology and models that are based on Coulomb friction are able to predict the energy dissipation along the rough surface. However, they fail to capture the transient from static to a flowing behaviour, and again when it ceases to flow. In large scale granular flow down slopes, only those grains that are located on the flow surface will have higher I values, due to lower mean pressures. However, grains located within the main flowing mass would experience higher mean pressure thus resulting in smaller I values. Hence, $\mu(I)$ rheology is less effective in large scale problems and a simple Mohr-Coulomb model will yield a similar response. It can be suggested that the flow is governed by its momentum. It is important to carry out DEM simulations to understand the mechanics of the flow transition behaviour. This will enable us to describe the continuum response of phase transition more efficiently.

1.3.3 Saturated and submerged granular flows

Submarine mass movements pose a significant threat to off-shore structures, especially oil and gas platforms. Geophysical hazards, such as debris flows and submarine landslides, usually involve flow of granular solids and water as a single-phase system. Modelling

the multi-phase interaction poses a serious challenge. The momentum transfer between the discrete and the continuous phases significantly affects the dynamics of the flow as a whole (Topin et al., 2011). The complex interactions between the soil and the ambient fluid is shown in figure 1.13. For a given granular mass, the energy balance can be written as

$$E_p + E_s = E_k + E_f + E_D + E_v + E_r, \quad (1.17)$$

where E_s is the seismic energy resulting from an earthquake, E_f is the friction loss, E_D the friction loss due to drag effects on the upper surface of the flow, E_v the loss due to viscous effects and E_r the energy used to remold or transform the intact material. During the course of a submarine slide event (or also a sub-aerial slide), there appears to be a process by which there are some changes in solid to water ratio which provides a sufficiently low strength to allow flow to take place (Locat and Lee, 2002). Whatever the exact nature of the phenomenon, it is embedded in the remoulding energy (E_r). In both sub-aerial and submarine landslides the triggering energy is the same (initial potential energy). It appears as though the submarine landslides experience more dissipation E_D and E_v than sub-aerial landslides, but one shouldn't prematurely conclude that the run-out in submarine landslide will be shorter due to more dissipation. The effect of hydroplaning and fluidisation of the flowing mass result in complex interactions, which makes it difficult to predict the exact mechanism of run-out and the length of run-out in submarine conditions for a given initial state.

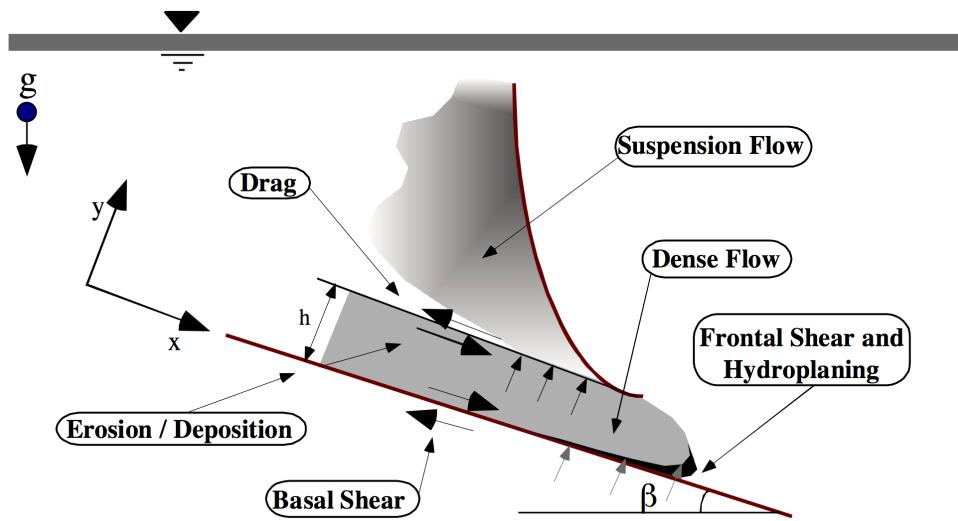


Figure 1.13 Schematic diagram showing the generation of a turbidity current (suspension flow) for drag forces on the surface, potential lifting of frontal lobe leading to the process of hydroplaning, the basal shear stress causing erosion and deposition (Locat and Lee, 2002).

Experimental findings

The collapse of a granular column, which mimics the collapse of a cliff, has been extensively studied in the case of dry granular material, when the interstitial fluid plays no role. The case of the collapse in presence of an interstitial fluid has been less studied (Topin et al., 2012). Rondon et al. (2011) performed granular column collapse experiments in fluid to understand the role of initial volume fraction. The experimental set-up of granular collapse in fluid performed by Rondon et al. (2011) is shown in figure 1.14.

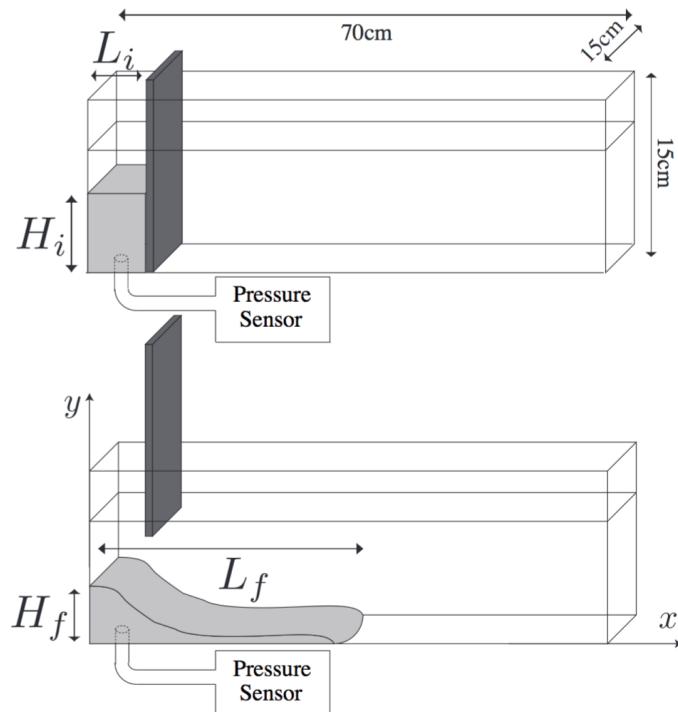


Figure 1.14 Experimental set-up of granular collapse in fluid (Rondon et al., 2011).

Figure 1.15 shows the evolution of run-out and pore-pressure at the bottom of the granular flow. The whole loose column is mobilised immediately, in contrast to the dense case. The loose column in fluid spreads almost twice than the dense case. The collapse of a granular column in a viscous fluid is found to be mainly controlled by the initial volume fraction and not by the aspect ratio of the column. The role of the initial volume fraction observed in the viscous collapse can be understood by the pore pressure feedback mechanism proposed by (Iverson, 2000; Schaeffer and Iverson, 2008) in the context of landslides.

Iverson (2000) observed in the large-scale field tests that the soil prepared in a loose state on a slope and subjected to a rainfall flows rapidly like a liquid when it breaks, whereas a dense soil only slowly creeps (figure 1.16). The underlying mechanism is related to the

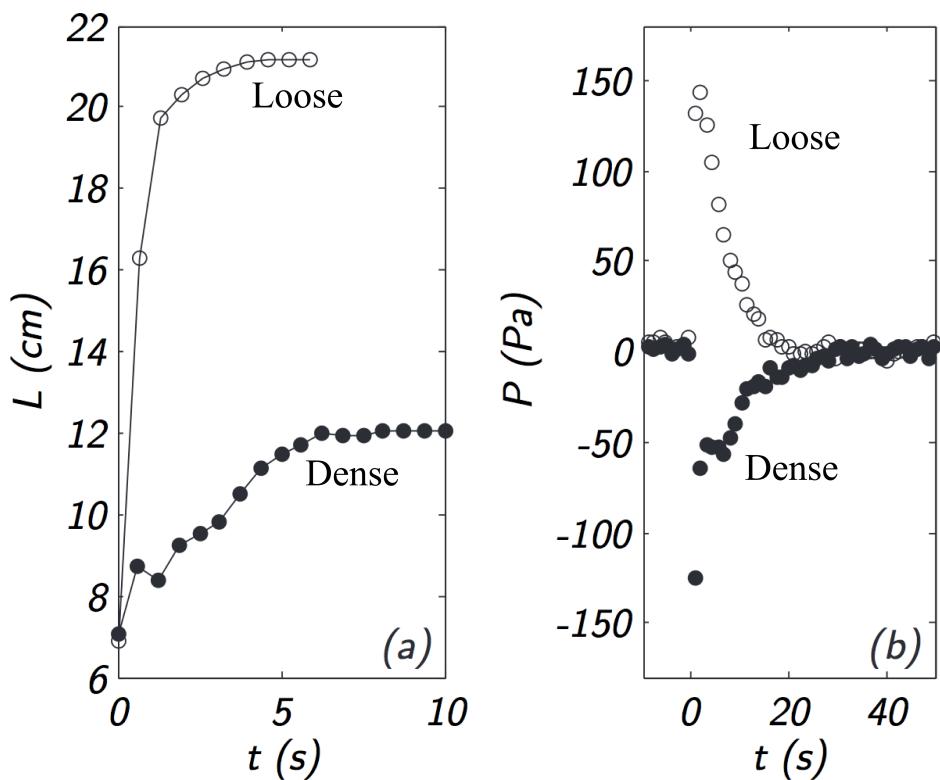


Figure 1.15 Evolution of run-out and pore-water pressure at the bottom for granular column collapse in fluid for dense and loose conditions (Rondon et al., 2011).

dilation or contraction character of the granular material, which the authors described as the “pore pressure feedback”. The compaction or dilation of grains can cause additional stress in the grains which can stabilise or destabilise the soil. The loose sediment experience high positive pore-pressure and low shear stresses resulting in a quicker flow, while the large negative pore-pressure in the dense case delays the run-out. The flow is controlled by the coupling between the dilatancy of the granular layer and the development of pore pressure in the fluid phase (Pailha et al., 2008).

The dense column needs to dilate in order to flow. When it starts to fall, liquid is then sucked into the column, which is then stabilized by the additional viscous drag (Rondon et al., 2011; Topin et al., 2012). In the dense condition, large negative-pore pressures are developed in the initial stages of collapse, they collapse has to overcome the large negative pore-pressure before it starts to flow. This results in a slow flow evolution as seen by the flatness of the initial run-out curve in dense condition in comparison to the steep slope in the loose case (figure 1.15). By opposition the loose column when it starts flowing expands and ejects liquid, leading to a partial fluidisation of the material. The large positive pore-pressure developed at the bottom of the flow in loose condition indicates water entrainment and hydroplaning. The entrainment of water at the basal flow front lubricates the frictional effect and along with hydroplaning it results in longer run-out distance.

Very few research has been carried out to understand the difference in mechanism of dry and submerged granular flow. Cassar et al. (2005) carried out experimental investigation on the flow of dense granular material down an inclined plane fully-immersed in water. The velocities observed in the submarine case were found to be a magnitude smaller than the dry condition. This is in contrast to the idea that the submarine landslides tend to flow longer than its sub-aerial counterpart. In order to compare the dry collapse with the submarine collapse, it is important to start with the same initial configuration. Packing soil grains to the same initial density is difficult. Hence, it is important to perform numerical studies and develop theoretical framework that can explain the submarine granular flow behaviour.

Numerical modelling

Although certain macroscopic models are able to capture simple mechanical behaviours, the complex physical mechanisms occurring at the grain scale, such as hydrodynamic instabilities, formation of clusters, collapse, and transport (Peker and Helvacı, 2007; Topin et al., 2011), have largely been ignored. In particular, when the solid phase reaches a high volume fraction, the strong heterogeneity arising from the contact forces between the grains, and the hydrodynamic forces, are difficult to integrate into the homogenization process involving global averages (Topin et al., 2011).

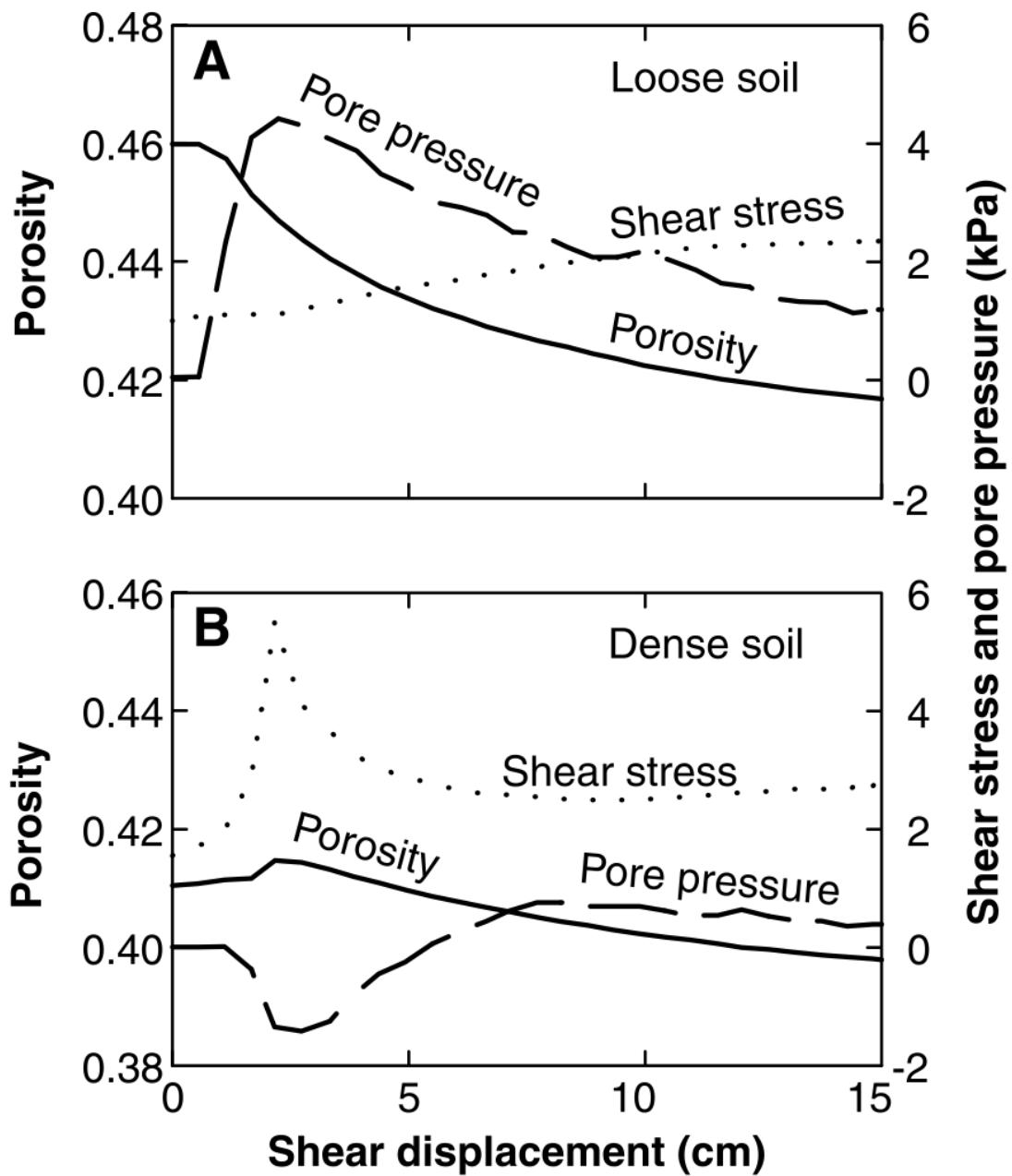


Figure 1.16 Pore pressure feedback mechanism: effect of density (Iverson, 2000).

In two-phase models (Pitman and Le, 2005), the momentum transfer between the grains and the suspension fluid depends on the momentum equations of both the phases. In case of mixture theory based models (Meruane et al., 2010), the shear-induced migration and grains collisions are considered in an average sense. In order to describe the mechanism of saturated and/or immersed granular flows, it is important to consider both the dynamics of the solid phase and the role of the ambient fluid (Denlinger and Iverson, 2001; Iverson, 1997). The dynamics of the solid phase alone are insufficient to describe the mechanism of granular flow in a fluid; it is important to consider the effect of hydrodynamic forces that reduce the weight of the solids inducing a transition from dense-compacted to dense-suspended flows, and the drag interactions which counteract the movement of the solids (Meruane et al., 2010).

Topin et al. (2011) performed granular collapse in fluid using Non-Smooth Contact Dynamics coupled with distributed Lagrange multiplier/fictitious domain (DLM/FD) method. The mechanism of collapse of granular columns in dry and submerged conditions were compared. Topin et al. (2011) observed that for a given initial geometry the run-out distance in the dry case is significantly higher than the submerged condition, this observation is similar to the experimental results of Cassar et al. (2005). In the dry case, inertia is responsible for the enhanced mobility at high aspect ratio. However in submerged conditions, i.e., in the viscous regime, the inertial effects remain negligible, which could explain why the important parameter controlling the dynamics is the initial volume fraction and not the initial aspect ratio. Topin et al. (2011) observed that the run-out exhibit a power-law relation with the peak kinetic energy and the largest value of run-out in fluid inertial regime, and the lowest in grain-inertial and intermediate value for the viscous-regime (figure 1.17). The viscous regime is where the grain reaches the viscous limit velocity, the Stoke's number $S_t \ll 1$ and the density ratio $r \gg S_t$ (Courrech du Pont et al., 2003). However, the role of the volume fraction on dry granular collapse has not been precisely studied and the preparation of the pile may also play a role Daerr and Douad (1999).

The $\mu(I)$ rheology relates the non-dimensionless number I to the shear rate through a characteristic time. In the case of dry granular flows, the parameter I is defined as the ratio between the time taken for a grain to fall into the hole, t_{micro} , and the meantime, t_{mean} , which is inversely related to the shear rate. Cassar et al. (2005) observed that the run-out behaviour collapse on to a single friction law, which shows that the major role of the fluid is to change the time it takes for a grain to fall into a void-space. The $\mu(I)$ rheology for dry dense flows can be modified to capture the behaviour of dense submarine granular flows, if the inertial time scale in the rheology is replaced with a viscous time scale. Pitman and Le (2005) observed that if the fluid inertial effects are small enough, then a simpler model can be adopted. Sketch of the motion of a grain $z(t)$ during a simple shear $\dot{\gamma}$ under a confining

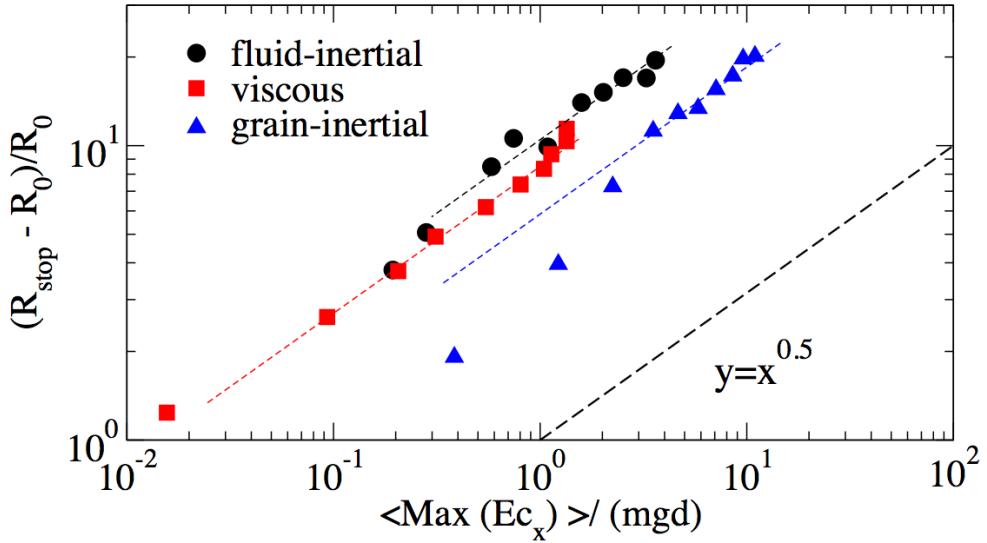


Figure 1.17 Normalised run-out distance as a function of the peak value of the horizontal kinetic energy per grain. (Topin et al., 2011).

pressure P_g is shown in figure 1.18. Hence, assuming that the fluid velocity is low enough for the contact interaction between grains to be significant, the time taken by the grain to fall into a hole, t_{micro} , is then controlled by the viscosity of the ambient fluid. Thus, the dimensionless parameter can be modified to incorporate the viscous time to describe granular flow in a fluid (Pouliquen et al., 2005). In short time scales, the grain initially accelerates but because of the drag force, the grain eventually reaches a limit viscous velocity $v_{\infty v}$. The time required to travel a diameter d is given as $t_{fall} = d/v_{\infty v}$. This new viscous time is used to define the dimensionless number.

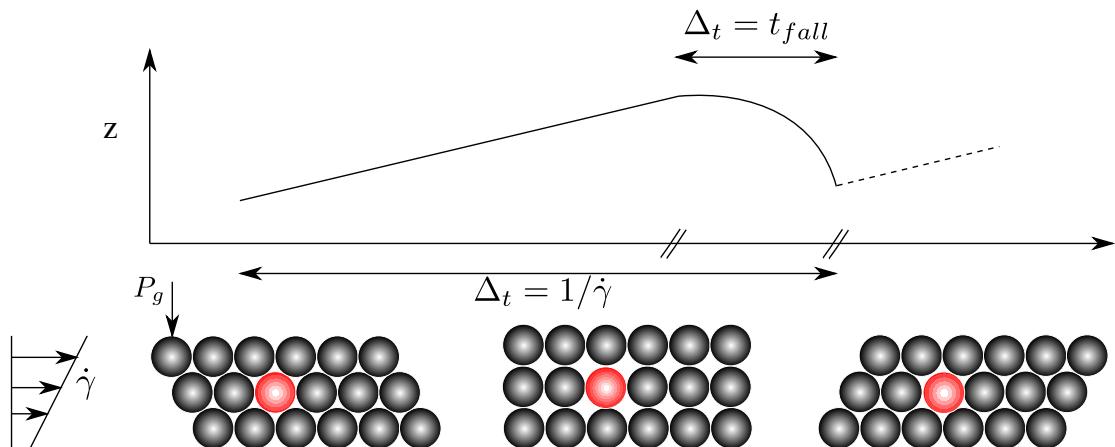


Figure 1.18 Sketch of the motion of a grain $z(t)$ during a simple shear $\dot{\gamma}$ under a confining pressure P_g .

Comments on modelling

The $\mu(I)$ rheology is found to be valid only for the steady uniform regime; unsteady phenomena such as the triggering of avalanches result in coupling between the granular grains and the ambient fluid, which are much more complex to model. Transient regimes characterized by change in solid fraction, dilation at the onset of flow and development of excess pore pressure, result in altering the balance between the stress carried by the fluid and that carried by the grains, thereby changing the overall behaviour of the flow (Denlinger and Iverson, 2001). The $\mu(I)$ rheology seems to predict well the flow of granular materials in the dense regime. However, the transition to the quasi-static regime where the shear rate vanishes is not captured by the simple model. Also, shear band formation observed under certain flow configurations is not predicted. The flow threshold or the hysteresis characterizing the flow or no-flow condition is not correctly captured by the model, which can be due to the discrepancies between the physical mechanism controlling the grain level interactions, clustering, and vortex formations. When the scale of the system is larger than the size of the structure, a simple rheology is expected to capture the overall flow behaviour, however the size of the correlated motion is the same as that of the system, causing difficulties in modelling the flow behaviour (Pouliquen et al., 2005). Hence, it is essential to study the behaviour of granular flows at various scales, i.e. microscopic, meso-scale and at continuum level, in order to develop a constitutive model that captures the entire flow process.

1.4 Summary

Granular flow involves three distinct regimes: the dense quasi-static regime, the rapid and dilute flow regime, and an intermediate regime. The dynamics of homogeneous granular flow also involve at least three different scales, making it difficult to describe the mechanics of granular flow by simple theories. It is important to describe the granular dynamics as an initial-value problem. Experimental conditions are too difficult to reproduce precisely, resulting in inherent inconsistencies in the results. Numerical models, such as the shallow-water approximation, kinetic theory approach, and rheologies have captured the basic flow dynamics, but have failed to describe the complete mechanics of the granular flow.

Collapse of a granular column is a simple case of granular flow. Experimental results have shown that the run-out exhibit a power-law dependence with the initial aspect ratio of the column. Although, numerical simulations and theoretical frameworks were able to recover the power-law behaviour, they were unable to explain the origin of the power law or capture the various stages of the flow. The initial conditions have a significant impact on the overall behaviour of the granular system, however, a theoretical framework that is capable

of describing the influence of material properties on the run-out behaviour is still lacking. In the present study the capability of continuum models such as the Mohr-Coulomb model and $\mu(I)$ rheology in modelling the granular column collapse is investigated by comparing it with the discrete-element simulations. The role of initial packing fraction on the run-out behaviour is also investigated in the present study.

Submarine granular flows exhibit complex interactions between the soil grains and the ambient fluid. The presence of fluid causes drag which slows down the run-out, while the entrainment at the flow front causes hydroplaning and longer run-out distance. The run-out distance is found to be controlled by the initial volume rather than the aspect ratio of the column. Loose granular column is found to flow longer than the dense condition. However, researchers observed longer run-out in dry condition in comparison with the submerged collapse. The difference in the mechanism of dry and submerged granular flows is not well researched. The role of initial volume fraction on the run-out behaviour is not precisely known. This study focuses on the effect of initial packing and permeability on the run-out by performing grain-scale simulations. This study investigates the influence of grain-scale quantities, which are otherwise not accessible experimentally, on the run-out behaviour thus providing useful insight into the flow dynamics, thereby enabling us to develop better constitutive laws.

Chapter 2

Numerical modelling of granular flow

2.1 Introduction

Most geotechnical analyses involve failure prediction and design of structures that can safely withstand applied loads. However, it is very important to study the post-failure behaviour to mitigate risk posed by geophysical and gravity-driven flows such as landslides, avalanches, slope failures, and debris flows. Granular flows are complex problems in continuum mechanics for which no closed-form solution exists. Hence it is essential to develop alternative solution schemes, which are capable of simulating failure mechanisms and post-failure dynamics of granular media.

The dynamics of a homogeneous granular flow involves at least three distinct scales: the *microscopic scale*, which is characterised by the contact between grains, the *meso-scale* that represents micro-structural effects such as grain rearrangement, and the *macroscopic scale*, where geometric correlations can be observed (figure 2.1). Conventionally, granular flows are modelled as continua because they exhibit many collective phenomena. However, on a grain scale, granular materials exhibit complex solid-like and/or fluid-like behaviour. Recent studies, however, suggest that a continuum law may be unable to capture the effect of inhomogeneities at the grain scale level, such as orientation of force chains, which are micro-structural effects. Discrete element methods (DEM) are capable of simulating these micro-structural effects, however they are computationally expensive.

2.2 Continuum modelling of granular flow

The most powerful way of modelling the granular assembly is through numerical techniques. It is important to argue why it is acceptable to model the granular materials as a contin-

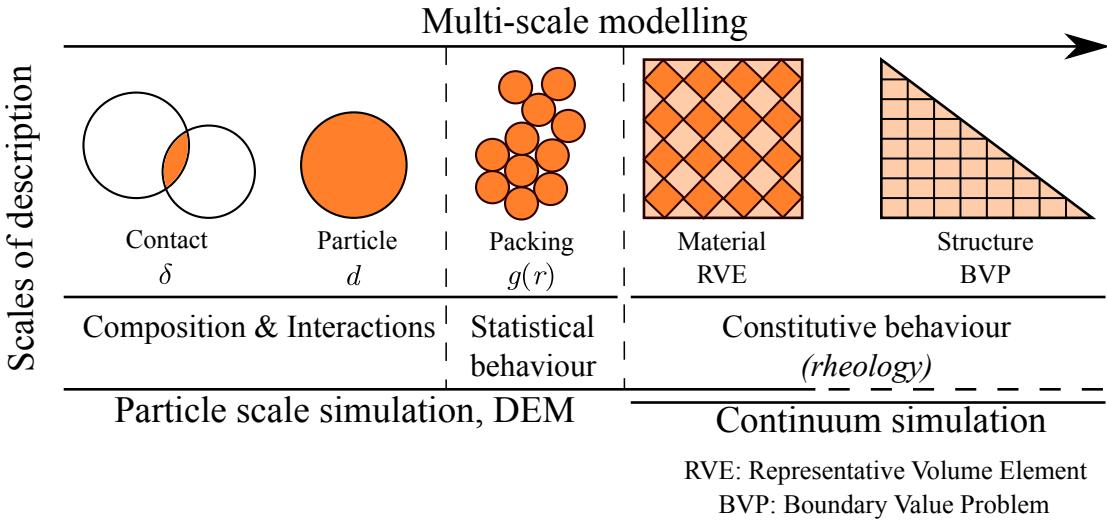


Figure 2.1 Schematic representation of different scales of description involved in the multi-scale modelling of granular materials

uum. Even at the outset, it may appear that such a treatment is objectionable for some reason. The most obvious is the fact that the micro-constituents of granular matter, i.e. the individual grains, are not small enough to warrant a continuum description (Kamrin et al., 2007). Typical continuum laws are only expected to apply when there is a strong separation of scales, i.e. separation of the micro-scale from the macro-scale, in the flow geometry. Continuum mechanics relies on the fundamental notion of a representative volume element, in which properties averaged over discrete grains exhibit deterministic relationships. Recent work on granular materials suggests that a continuum law may be incapable of revealing inhomogeneities at the grain-scale level (Rycroft et al., 2009). Microscopic features of dense granular materials, which seem to defy a simple continuum description include (i) complex, fractal networks of force chains, which are inhomogeneous down to the grain level (Goldhirsch, 2003), (ii) buckling of force chains and instabilities in shear band, (iii) anomalous, non-collisional particle dynamics and proximity to the jamming transition, where geometrical packing constraints suppress any dynamics, and (iv) wide range of dynamic response, from liquid-like to solid-like behaviour (Aranson and Tsimring, 2001, 2002; Jaeger et al., 1996). The first three points cast serious doubt on the prospects of a continuum law. The third point means that the full stress tensor must be described, and it may depend on strain, deformation rate, and material variables that can evolve during the process (Rycroft et al., 2009).

Granular materials exhibit many collective phenomena (Jaeger et al., 1996). However, no continuum model is yet capable of describing behaviours such as granular fingering on rough slopes, plug flow and the occurrence of localized shear bands in the granular materials.

Most constitutive models, even in the simple case of dry granular flows, cannot describe the entire range of flow from solid to fluid. In certain cases, granular flow is modelled as a fluid behaviour. Continuum models that are based on averaging techniques applied to representative volume elements are mostly utilised in problems involving quasi-static conditions. The fundamental question is how to meaningfully model granular materials which exhibit complex phenomena.

The oldest approach involves modelling the granular material as a rigid solid, which behaves as an ideal Coulomb material and undergoes failure if the ratio of the shear stress to the normal stress in any plane reaches a critical value of the Coulomb internal friction coefficient μ . The stress is determined based on the mechanical equilibrium of the system along with the hypothesis of *incipient yield*, i.e. the yield criterion is attained everywhere at all times (in a “*limit-state*”) (Rycroft et al., 2009). The fundamental assumption of a limit-state stress field at incipient yield everywhere is questionable. Granular flows can contain regions of stress lying within the yield surface. In fact, discrete-element simulations show that the grains in this region essentially remain static (Staron et al., 2005). Some of the limitations of the Mohr-Coulomb plasticity in modelling granular materials include: linearisation of limit-stress envelope, inability to account for variable volume change characteristics depending on pre-consolidation pressure during shearing, predicting unrealistic negative pore-pressure upon shearing due to constant rate of dilation, and inability to predict compressive plastic strains in soft-soils. Mohr–Coulomb plasticity has been used extensively in engineering applications (Nedderman, 1992), but the general solution requires sophisticated numerical techniques to capture shock-like discontinuities in stress and velocity, which arise even in relatively simple geometries.

The coaxiality feature of Mohr-Coulomb plasticity is useful in describing debris flows. The principle of coaxiality claims that material should flow by extending along the minor principal stress direction and contracting along the major principal stress direction; the principal planes of stress are aligned with the principal planes of strain-rate. Granular materials deform solely based on the alignment of the principal planes. Under this assumption, the major principal plane is usually vertical due to gravity, and the coaxiality rule requires the material to expand horizontally, which is the case for granular column collapse. However, the coaxiality can be troubling depending on the circumstances. Suppose we have a flat-bottomed quasi-2D silo with smooth side-walls. Under standard filling procedures, the walls provide only enough pressure to keep the grains from sliding farther out. For example, in a slow dense granular flow through a silo, the principal plane remains vertical and coaxiality requires the granular material to expand horizontally, thus making it geometrically impossible for the granular material to converge and exit through the orifice. Depending on the boundary

conditions, Mohr-Coulomb plasticity can result in discontinuities or jumps in the velocity and stress fields (Rycroft et al., 2006). Coaxiality can also violate principles of thermodynamics. Coaxiality only ensures there is no shear strain-rate in the principal stress reference frame and actually does not directly enforce that of the two principal strain-rate axes, the axis of maximal compression (i.e. the major principal strain-rate direction) must align with the major principal stress direction.

Roscoe (1970) showed that the principal axes of strain rate and of stress are generally not coincident during simple shear tests of sand. Despite the plastic character of the flow, the flow rules obtained by employing the rheological concept of perfect plasticity to granular materials (perfect soil plasticity) are definitely inadequate for a description of fully developed shear flow. The non-coaxiality of the tensors of stress and strain increment is able to explain the shear flow behaviour. The rotations of the principal stress and the principal plastic strain rate are found to be non-coaxial particularly at the early stage of loading. However, the axes tend to become coincident at large shear strains (Yu and Yuan, 2006), which are common in geophysical flows.

Advanced elasto-plastic models based on the *critical state* theory provide a better representation of granular flows in a quasi-static regime, but do not have any rate-dependent effects that are associated with rapid granular flows. At large shear strains, such as geophysical flows, the granular mass is considered to be in critical state. Another continuum based model is the partial fluidisation model, which uses a set of equations that describes the flow velocity and the shear stresses along with an auxiliary order parameter to predict granular flow behaviour. The order parameter of the granular media controls the size of the viscous-like contribution to the stress tensor, and describes the transition between the flowing and the static components of the granular system (Aranson and Tsimring, 2001). A constitutive model, which considers the solid fraction as the main microscopic parameter for describing dense granular flow was proposed by Josserand et al. (2004). The stress in the granular material is divided into a rate-dependent part representing the rebound-less impact between grains, and a rate-independent part associated with longer contacts, i.e. quasi-static regime. Although, the model captures shear localization behaviour, it fails to describe granular flow behaviour at rough boundaries. In the basal or frictional layer, grain rotation plays an important role. This causes the grain stress tensor to be non-symmetric and results in a perturbed profile in the solid fraction, these phenomena would require specific modelling (Josserand et al., 2004).

In the case of saturated/submerged soil conditions, most continuum techniques do not consider fully coupled behaviour. Instead, they consider the soil-fluid mixture as a single phase material. However, modelling of pore pressure dissipation is important to capture accurate flow behaviour, especially in submarine conditions, where they play a crucial role

in the flow dynamics. Presence of ambient fluid may retard the flow due to viscous drag or accelerate the flow through a lubrication effect. Fully coupled constitutive models are essential to realistically capture the initiation and propagation of rapid granular flows.

Granular materials are composed of distinct grains, which interact only at the contact points. It is assumed that the deformations of individual grains are negligible in comparison with the deformation of the granular assembly as a whole. The latter deformation is primarily due to the movement of the grains as rigid bodies. Therefore, it can be argued that precise modelling of grain deformation is not necessary to obtain a good approximation of the overall mechanical behaviour. An Eulerian grain-level continuum model describes the response of individual grains to the applied loads. However, continuum mechanics solves over the whole domain using initial and boundary conditions appropriate for the problem. Hence, continuum models are still widely used to solve engineering problems associated with granular materials and flows.

2.2.1 Mesh-based and mesh-free techniques

In continuum mechanics, there are two different view points describing the deformation of a continuum, namely Lagrangian and Eulerian descriptions. In the Lagrangian description the movement of the continuum is specified as a function of the material coordinates and time. This is a particle description that is often applied in solid mechanics. On the other hand, the Eulerian description focuses on the current configuration, giving attention to what is occurring at a fixed point in space as time progresses, instead of giving attention to individual particles as they move through space and time. The Eulerian description is commonly used for describing fluid flows where kinematic properties are of great interest.

Conventional mesh based Lagragian approaches, such as the Finite Element Method or the Finite Difference Method are capable of modelling history-dependent material behaviour and have well-defined free surfaces. However, they require complex re-meshing and remapping of variables, which cause additional errors in simulating large deformation problems (Li and Liu, 2002). Unlike Lagrangian FEM, in Eulerian FEM the computational mesh is kept spatially fixed while the material is deforming in time. This allows the capability of handling large deformation without the problem of mesh distortion. As the computational mesh is completely decoupled from the material, convective terms appear in Eulerian FEM, introducing numerical difficulties because of their non-symmetrical properties (Donea et al., 1982). Additionally, Eulerian FEM is difficult to use with history-dependent constitutive models. The Coupled Eulerian–Lagrangian (CEL) method is an arbitrary Lagrangian-Eulerian method that attempts to capture the advantages of both the Lagrangian and the Eulerian method in modelling large deformation problems in geomechanics (Qiu et al., 2011). This approach involves solving the

governing equations in a Lagrangian step, thus obtaining the material displacement, followed by the Eulerian step where a new mesh is generated and the variables are transferred to the new mesh. This requires more computation time.

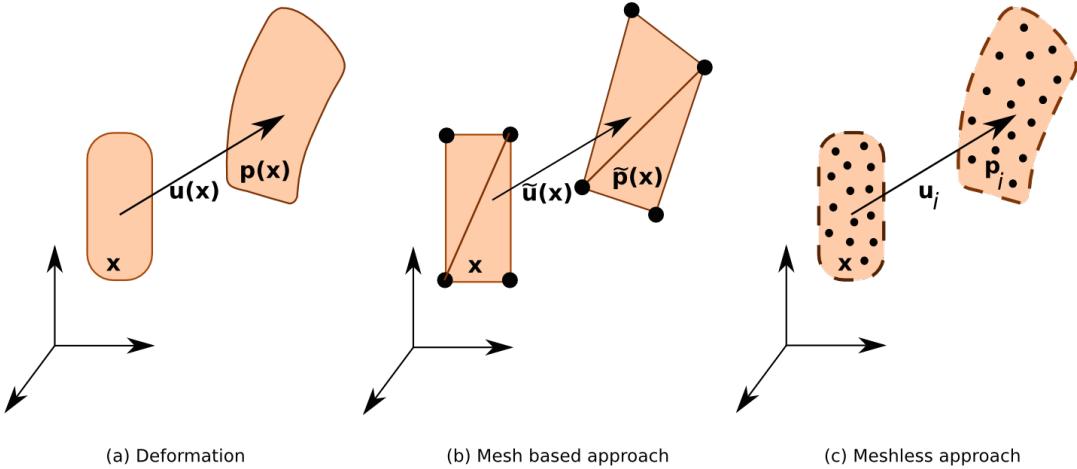


Figure 2.2 Difference between mesh-based and mesh-free techniques in modelling large deformation flow.

An alternative to the mesh-based approach is using mesh-less Lagrangian methods (figure 2.2) where the nodes representing the solids transform as the continuum deforms, avoiding the problem of mesh distortion, i.e., the nodes representing the solids can move freely within the domain. Mesh free methods such as Smooth Particle Hydrodynamics and Material Point Method are not constrained by the mesh size and mesh distortion effects, and hence can be effectively used in simulating large deformation problems, such as debris flow and submarine landslides.

The element-free Galerkin (EFG) method is a relatively new mesh-less method, in which the trial functions for the weak form are constructed using moving least squares interpolation (Belytschko et al., 1994). The particle finite element method (PFEM) is another mesh-less method that involves mesh-less finite element interpolation. In PFEM, the nodal points represent the particles and the computational mesh is constructed by connecting these points. The mesh is then used to solve the governing equations in a Lagrangian fashion. In PFEM, large deformation requires frequent re-meshing (Kafaji, 2013).

Smooth Particle Hydrodynamics is the oldest mesh-free technique, in which the domain is discretised into particles that have a spatial distance, called the *smoothing length* over which the material properties are “smoothed” by a kernel function. SPH was developed to solve astrophysical problems (Monaghan, 2005). SPH has been applied in geomechanics for solving large deformation problems (Augarde and Heaney, 2009; Maeda and Sakai, 2010;

Mori, 2008). Although SPH has been successfully used, it has a few drawbacks: SPH exhibits spatial instabilities, as a consequence of the point-wise integration (Bonet and Kulasegaram, 2000), insufficient neighbouring particles causes inconsistencies, and it is computationally expensive as a result of the search for the neighbouring particles (Bandara, 2013).

2.3 Material Point Method (MPM)

The Material Point Method (MPM) (Sulsky et al., 1994, 1995) is a particle based method that represents the material as a collection of *material points*, and their deformations are determined by *Newton's laws of motion*. Sulsky et al. (1994) extended the Particle-in-Cell (PIC) method (Harlow, 1964) to computational solid mechanics by taking advantage of the combined Eulerian-Lagrangian approach. The Material Point Method is a hybrid Eulerian-Lagrangian approach, which uses moving material points, and computational nodes on a background mesh. This approach is very effective particularly in the context of large deformations (Andersen and Andersen, 2010; Bandara, 2013; Mackenzie-Helnwein et al., 2010; Mast et al., 2014a; Shin, 2010; Zhang et al., 2009). Although, not derived directly from what is classically considered as mesh-free or mesh-less methods, MPM is still considered as a mesh-free approach, primarily because the initial discretisation of the material does not involve a polygonal tessellation, as in the Finite Element Method. However, MPM utilizes a background mesh to perform differentiation, integration, and to solve equations of motion (Steffen et al., 2008). The background mesh can be of any form, however for computational efficiency a Cartesian lattice is adopted.

A typical 2D discretisation of a solid body is shown in figure 2.3. The grey circles in figure 2.3 are the material points x_p , where 'p' represents a material point, and the computational nodes are the points of intersection of the grid (denoted as X_i , where i represents a computational node). MPM involves discretising the domain Ω with a set of material points. The material points are assigned an initial value of position, velocity, mass, volume, and stress denoted as \mathbf{x}_p , v_p , m_p , \mathbf{V}_p and σ_p . Depending on the material being simulated, additional parameters, like pressure, temperature, pore-water pressure, etc., are specified at the material points. The material points are assumed to be within the computational grid which for, ease of computation, is assumed to be a Cartesian lattice (figure 2.3). At every time step t_k , the MPM computation cycle involves projecting the data, such as position, mass, and velocity from the material points to the computational grid using the standard nodal basis functions, called the *shape functions*, derived based on the position of particle with respect to the grid. Gradient terms are calculated on the computational grid and the governing equation, i.e. the equation of motion, is solved and the updated position

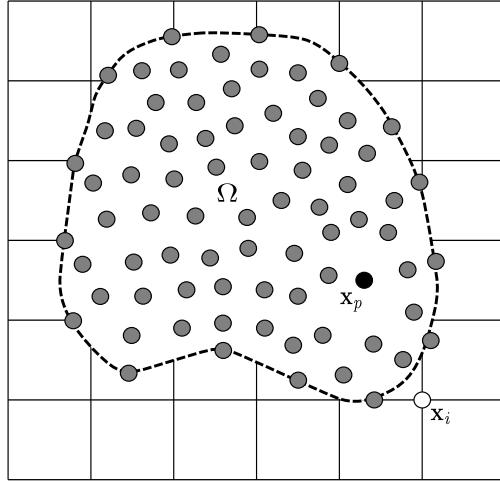


Figure 2.3 Typical discretisation of a domain in MPM. The dotted line represents the boundary of the simulated object Ω and each closed point represents a material point used to discretise Ω . The square mesh represents the background grid. Each square in the background grid is a grid cell, and grid nodes are located at the corners of grid cells.

and velocity values are mapped back to the material points. The mesh is reinitialized to its original state and the computational cycle is repeated.

2.3.1 Discrete formulation of the governing equations

The governing differential equation for a continuum is derived from the conservation of mass and momentum:

$$\frac{\partial \rho}{\partial t} \rho \Delta \cdot v = 0, \quad (2.1)$$

$$\rho a = \Delta \cdot \sigma + \rho b, \quad (2.2)$$

where $\rho(\mathbf{x}, t)$ is the mass density, $\mathbf{v}(\mathbf{x}, t)$ is the velocity, $\mathbf{a}(\mathbf{x}, t)$ is the acceleration, $\sigma(\mathbf{x}, t)$ is the Cauchy's stress tensor, and $\mathbf{b}(\mathbf{x}, t)$ is the body force. The vector \mathbf{x} represents the current position of any material point in the continuum, at time t . In MPM, the continuum body is discretised into a finite number of material points N_p . Let \mathbf{x}_p^t ($p = 1, 2, \dots, N_p$) denote the current position of material point p at time t . Each material point, at any given time t , has an associated mass m_p^t , density ρ_p^t , velocity v_p^t , Cauchy stress tensor σ_p^t , strain ϵ_p^t , and other necessary internal state variables based on the adopted constitutive model. These material points provide a Lagrangian description of the continuum body; since material points have a fixed mass at all times, eq. 2.1 is satisfied. The data from the material points are mapped on to the nodes of the computational grid, where the discrete form of eq. 2.2 is described. The

weak form of eq. 2.2 is obtained by multiplying eq. 2.2 with a test function $w(\mathbf{x}, t)$:

$$\int_{\Omega} \rho \mathbf{w} \cdot \mathbf{a} d\Omega = - \int_{\Omega} \rho \sigma^s : \Delta \mathbf{w} d\Omega + \int_{\partial\Omega_t} w \cdot \tau dS + \int_{\Omega} \rho w \cdot \mathbf{b} d\Omega, \quad (2.3)$$

where σ^s is the specific stress (i.e. stress divided by mass density, $\sigma^s = \sigma/\rho$), Ω is the current configuration of the continuum, τ is the surface traction. Eq 2.3 is obtained by applying the divergence theorem, similar to the standard procedure adopted in Finite Element Methods (Chen and Brannon, 2002; Sulsky et al., 1994, 1995). The differential volume and the surface elements are denoted by $d\Omega$ and dS , respectively.

As the whole continuum is discretised into a finite set of material points, the mass density can be written as

$$\rho(\mathbf{x}, t) = \sum_{p=1}^{N_p} m_p \delta(x - x_p^t), \quad (2.4)$$

where δ is the Dirac delta function. Substituting eq. 2.4 in eq. 2.3, the sum of quantities of material points can be evaluated as

$$\begin{aligned} \sum_{p=1}^{N_p} m_p [w(x_p^t, t) \cdot \mathbf{a}(x_p^t, t)] &= \sum_{p=1}^{N_p} m_p [-\sigma^s(x_p^t, t) : \Delta w|_{x_p^t} \\ &\quad + w(x_p^t, t) \cdot \tau^s(x_p^t, t) h^{-1} + w(x_p^t, t) \cdot \mathbf{b}(x_p^t, t)], \end{aligned} \quad (2.5)$$

where h is the thickness of the boundary layer upon which the traction boundary conditions are enforced. Since the continuum body is moving in an arbitrary computational mesh, all the boundary conditions are carried by the boundary particles. If only one boundary particle is located in a cell, the cell boundary becomes a part of the continuum boundary, and the cell size represents the thickness of boundary layer. If both boundary and interior particles of the continuum are located in a cell, this cell becomes a mixed one. However, the mixed cell is still treated as a boundary cell. In other words, the interior particles temporarily become boundary ones. To avoid numerical errors, therefore, small cells must be used to contain only boundary particles if possible, and the boundary conditions are enforced in each time step.

It can be noted from eq. 2.5 that the interactions between different material points are reflected only through the gradient terms. In MPM, a background computational mesh is used to calculate the gradient terms. The computational mesh is constructed using 2-node cells for 1-D, 4-node cells for 2-D, and 8-node cells for 3-D problems. These elements are used to define the standard nodal basis functions, $N_i(\mathbf{x})$, associated with the spatial nodes $x_i(t), i = 1, 2, \dots, N_n$, where N_n represents the total number of mesh nodes. The nodal basis functions are assembled by using the conventional finite-element shape functions (Chen and

Brannon, 2002). The co-ordinates of any material point in a cell can be represented by

$$x_p^t = \sum_{i=1}^{N_n} x_i^t N_i(\mathbf{x}_p^t). \quad (2.6)$$

Similarly the nodal displacements, velocity and acceleration of any material point in a cell are represented using the basis functions. Thus, the test function has to be of the form

$$w_p^t = \sum_{i=1}^{N_n} w_i^t N_i(\mathbf{w}_p^t). \quad (2.7)$$

Equations (2.6) and (2.7) ensure that the associated vectors are continuous across the cell boundary. However, the gradient of these functions is not continuous, due to the use of linear shape functions. Substituting, eq. 2.6 and eq. 2.7 into eq. 2.5, the weak form of the equation of motion reduces to

$$\sum_{j=1}^{N_n} m_{ij}^t \mathbf{a}_j^t = \mathbf{f}_i^{int,t} + \mathbf{f}_i^{ext,t}, \quad (2.8)$$

where the nodal mass, m_{ij}^t is represented as

$$m_{ij}^t = \sum_{p=1}^{N_p} m_p N_i(x^t) N_j(x^t). \quad (2.9)$$

The nodal internal force, $\mathbf{f}_i^{int,t}$ and the nodal external force, $\mathbf{f}_i^{ext,t}$ are defined as

$$\begin{aligned} \mathbf{f}_i^{int,t} &= - \sum_{p=1}^{N_p} m_p \mathbf{G}_{ip}^t \cdot \boldsymbol{\sigma}_p^{s,t} \\ \mathbf{f}_i^{ext,t} &= - \sum_{p=1}^{N_p} m_p \mathbf{b}_p^t N_i(\mathbf{x}_p^t) + \sum_{p=1}^{N_p} m_p N_i(\mathbf{x}_p^t) \tau_p^{s,t} h^{-1} \end{aligned} \quad (2.10)$$

where $\mathbf{G}_{ip}^t = \Delta N_i(x)|_{x=X_p^t}$. The nodal accelerations are obtained by explicit time integration of eq. 2.8. To obtain stable solutions, the time step used in the analysis should be less than the critical time step, which is defined as the ratio of the smallest cell size to the wave speed (Chen and Brannon, 2002). The critical time increment is obtained as

$$\Delta t_{crit} = L/c, \quad (2.11)$$

$$c = \frac{K + \frac{4}{3}G}{\rho_s}, \quad (2.12)$$

where L is the background cell size, c is the pressure wave velocity, K and G are the bulk modulus and the shear modulus of the solid and ρ_s is the density of the soil skeleton. The boundary conditions are enforced on the cell nodes and the nodal velocities are obtained by solving the equation of motion at each node. The strain increment for each material point is determined using the gradients of the nodal basis functions. The corresponding stress increments are computed using the adopted constitutive law. After updating all the material points, the computational mesh is discarded, and a new mesh is defined for the next time step.

2.3.2 Boundary conditions

The Material Point Method uses standard shape functions, similar to those used in the Finite Element Methods, hence the essential and the natural boundary conditions can be applied to the background grid nodes in the same way as in the traditional FEM. The free surface boundary conditions are satisfied, as the MPM is formulated in the weak form. Implementation of traction boundary conditions requires a set of material points to represent the boundary layer. Bandara (2013) proposed a friction interaction for the planar boundary condition, using Coulomb's friction criterion. The friction boundary algorithm for the solid phase adopted in the present study is shown in algorithm 1. The friction boundary conditions are applied on the mesh nodes by controlling the nodal acceleration tangential to the boundary. The nodal accelerations are considered to include the frictional effects instead of the forces, as the forces are proportional to the corresponding accelerations. Both static and kinetic friction are considered, and are applied only when the particles are in contact with the boundary. The static and kinematic frictions are applied in the direction tangential to the nodal boundary. Friction forces are applied only if the particles are in contact. The normal velocity and acceleration on the boundary plane is zero. Displacement boundary conditions are applied as velocity constraints on the nodes in the background mesh.

2.3.3 Integration scheme

Love and Sulsky (2006) investigated the energy consistency of MPM and observed that the MPM algorithm is more suited to flow calculations than the Lagrangian finite element method. Since, energy consistent MPM formulation is effective in simulating materials that exhibit localised dissipative mechanisms. In dynamic MPM, an explicit time integration scheme is adopted to advance the solution. Bardenhagen (2002) studied the energy consistency of MPM using two different explicit integration schemes. The *update stress first* (USF) scheme involves updating the strain and the stress at the beginning of the time step from the velocities

Algorithm 1 Friction boundary algorithm for solid phase in MPM (Bandara, 2013)

```

if  $a_{sI,t}^{k+1} < 0.0$  then
     $v_{sI,t}^{k+1,tmp} = v_{sI,t}^k + \Delta a_{sI,t}^{k+1}$ 
    if  $v_{sI,t}^{k+1,tmp} = 0$  then                                 $\triangleright$  static friction condition
        if  $a_{sI,t}^{k+1} \leq \mu_s |a_{sI,n}^{k+1}|$  then
             $a_{sI,t}^{k+1} = 0.$ 
        else                                          $\triangleright$  friction acts in the direction opposite to the tangential force
             $a_{sI,t}^{k+1} = a_{sI,t}^{k+1} - \mu_s |a_{sI,n}^{k+1}| \frac{a_{sI,t}^{k+1}}{|a_{sI,n}^{k+1}|}$ 
        end if
    else                                          $\triangleright$  Kinetic friction condition
        if  $v_{sI,t}^{k+1} \leq \mu_k |a_{sI,n}^{k+1}| \Delta t$  then
             $a_{sI,t}^{k+1} = -\frac{v_{sI,t}^k}{\Delta t}$ 
        else                                          $\triangleright$  friction acts in the direction opposite to the movement
             $a_{sI,t}^{k+1} = a_{sI,t}^{k+1} - \mu_k |a_{sI,n}^{k+1}| \frac{v_{sI,t}^{k+1}}{|v_{sI,n}^{k+1}|}$ 
        end if
    end if
end if

```

of the previous time step. In the *update stress last* (USL) approach the updated particle momentums are used to calculate the nodal velocities, which are then used to update the particle strain and stress. Bardenhagen (2002) observed that the USL approach performed better than the USF. The USL approach dissipates the energy slowly, while the USF approach is found to gain energy (Kafaji, 2013). The USL approach yields almost the same result as using the central difference scheme that is second order in time (Wallstedt and Guilkey, 2008). The *update stress last* approach is used in the present study due to its dissipative nature, which is useful in modelling granular flow problems, and numerical stability.

In problems involving a slow rate of loading, i.e., quasi-static problems, the flow of the material is much slower than the speed of wave propagation in the material. Hence, employing an implicit time integration scheme reduces the computational time considerably (Kafaji, 2013). Guilkey and Weiss (2003) proposed an implicit time integration method for MPM using quasi-static governing equations, and the Newmark integration scheme. Love and Sulsky (2006) showed implicit time integration in MPM is unconditionally stable. Although, MPM does not suffer from the limitations of FEM in simulating large deformations, more research is required for applying implicit time integration for large deformation problems. The present study focuses on large deformation problems, hence an explicit time integration scheme with the USL approach is adopted.

2.3.4 Solution scheme

In the present study a template-based three-dimensional C++11 Material Point Method code, developed at the University of Cambridge, is modified and extended to study granular flow problems. The three-dimensional MPM code is parallelised to run on multi-core systems, thus improving the computational efficiency. The algorithm of the MPM code is improved to handle multi-body dynamics and interactions. A step-by-step solution scheme for Material Point Method implemented in the present study is described below:

- A continuum body is discretised into a finite set of material points corresponding to the original configuration of the body. The number of material points corresponds to the resolution of the mesh size adopted in Finite Element Method. The material points are followed throughout the deformation of the material, which gives a Lagrangian description of the motion.
- An arbitrary computational grid is initialized to describe the natural coordinates of the material points. For the purpose of simplicity, a Cartesian grid is usually adopted.
- The state variables (mass/density, velocity, strain, stress, other material parameter corresponding to the adopted constitutive relation) are initialized at every material point.
- The shape function $N_{ip}^t(x_p)$ and the gradient of the shape function G_{ip}^t for each material point is computed.
- The information and properties carried by each material point is projected on to the background mesh using the shape functions computed from the particle position.
- The nodal mass matrix is obtained as

$$m_i^t = \sum_{p=1}^{N_p} m_p N_{ip}^t(x_p^t), \quad (2.13)$$

where m_i^t is the mass at node i at time t , m_p the particle mass, N_i the shape function associated with node i , and x_p^t the location of the particle at time t .

- The nodal velocity is obtained by mapping the particle velocity to the nodes using the shape functions. If necessary, the boundary conditions for the nodal velocities are applied.

$$\mathbf{v}_i^t = \sum_{p=1}^{N_p} m_p \mathbf{v}_p^t N_{ip}^t(x_p^t) / m_i^t. \quad (2.14)$$

- The momentum balance equation for the solid phase is solved and the nodal acceleration is computed as

$$a_i^t = \frac{1}{m_i^t} \left(- \sum_{p=1}^{N_p} G_{ip}^t \sigma_p^t \Omega_p^t + \sum_{p=1}^{N_p} m_p^t \mathbf{b}_p^t N_{ip}^t(x_p^t) \right). \quad (2.15)$$

If necessary, the boundary conditions for the nodal accelerations are applied.

- The nodal velocity at the end of the Lagrangian time step (L) is obtained from the computed nodal acceleration as:

$$v_i^L = \mathbf{v}_i^t + a_i^t \Delta t. \quad (2.16)$$

where $\Delta t = (t+1) - t$.

- The particle position and its velocity are updated according to:

$$\begin{aligned} \mathbf{x}_p^{t+1} &= \mathbf{x}_p^t + \Delta t \sum_{i=1}^{N_n} v_i^L N_{ip}^t, \\ \mathbf{v}_p^{t+1} &= \mathbf{v}_p^t + \Delta t \sum_{i=1}^{N_n} a_i^t N_{ip}^t. \end{aligned} \quad (2.17)$$

- The strain increment $\Delta \epsilon_p^{t+1}$ for particle is then computed as

$$\Delta \epsilon_p^{t+1} = \frac{\Delta t}{2} \sum_{i=1}^{N_n} G_{ip}^t \mathbf{v}_i^t + (G_{ip}^t \mathbf{v}_i^t)^T. \quad (2.18)$$

- The stress increment for the particle $\Delta \sigma_p^{t+1}$ is computed from the strain increment using the constitutive model adopted in the simulation

$$\Delta \sigma_p^{t+1} = \mathbf{D} : \Delta \epsilon_p^{t+1}. \quad (2.19)$$

In large deformation problems, the Jaumann rate is used to update the effective stress of the solid particles

$$\sigma_p^{t+1} = \Delta t (\sigma_p^t - \mathbf{W}_p^t - \mathbf{W}_p^t \sigma_p^t) x + \mathbf{D} : \Delta \epsilon_p^{t+1}, \quad (2.20)$$

$$\mathbf{W}_p^t = \sum_{i=1}^{N_n} \left[\mathbf{G}_{ip}^t \mathbf{v}_i^t - (\mathbf{G}_{ip}^t \mathbf{v}_i^t)^T \right]. \quad (2.21)$$

- The stress and the strain of the material points are updated based on

$$\begin{aligned}\sigma_p^{t+1} &= \sigma_p^t + \Delta\sigma_p^{t+1}, \\ \epsilon_p^{t+1} &= \epsilon_p^t + \Delta\epsilon_p^{t+1}.\end{aligned}\quad (2.22)$$

- In large deformation the volume of solid material points Ω_p is updated using the determinant J of the deformation gradient \mathbf{F}_p^{t+1} :

$$\Omega_p^{t+1} = J\Omega_p^{t_0}. \quad (2.23)$$

- The material point density is then updated as

$$\rho_p^{t+1} = \frac{\rho_p^t}{\{1 + \text{tr}(\Delta\epsilon_p^{t+1})\}}. \quad (2.24)$$

- At the end of every time step, all the variables on the grid nodes are initialized to zero. The material points carry all the information about the solution and the computational grid is re-initialised for the next step.

Figure 2.4 illustrates the steps involved in a MPM analysis.

Post processing

The post-processing stage, as in any analysis, involves visualization and extraction of the data from the analysis. In mesh-less methods, like the material point method, structures are generally represented as points which describe a discrete region of the body. MPM facilitates representation of arbitrarily complex geometries and has advantages over strictly grid based methods especially in simulations involving large deformations (Bardenhagen et al., 2000). However, MPM poses a whole new set of visualization problem. It is essential to visualize the general configuration of the body as well as observe the finer details like the development of cracks or separation of chunks of material from the body. The body is discretised into conceptual material points, which carry all the relevant information of the corresponding segment. The unique qualities of MPM necessitate the need to visualize the particle data in a way that is informative and appropriate.

In MPM, the particle data represents the finite portion of a larger continuum, and the ability to see and interpret the macroscopic structure created by these particles is vital (Bigler et al., 2006). There are two main aspects in visualizing MPM data: (1) visualization of the

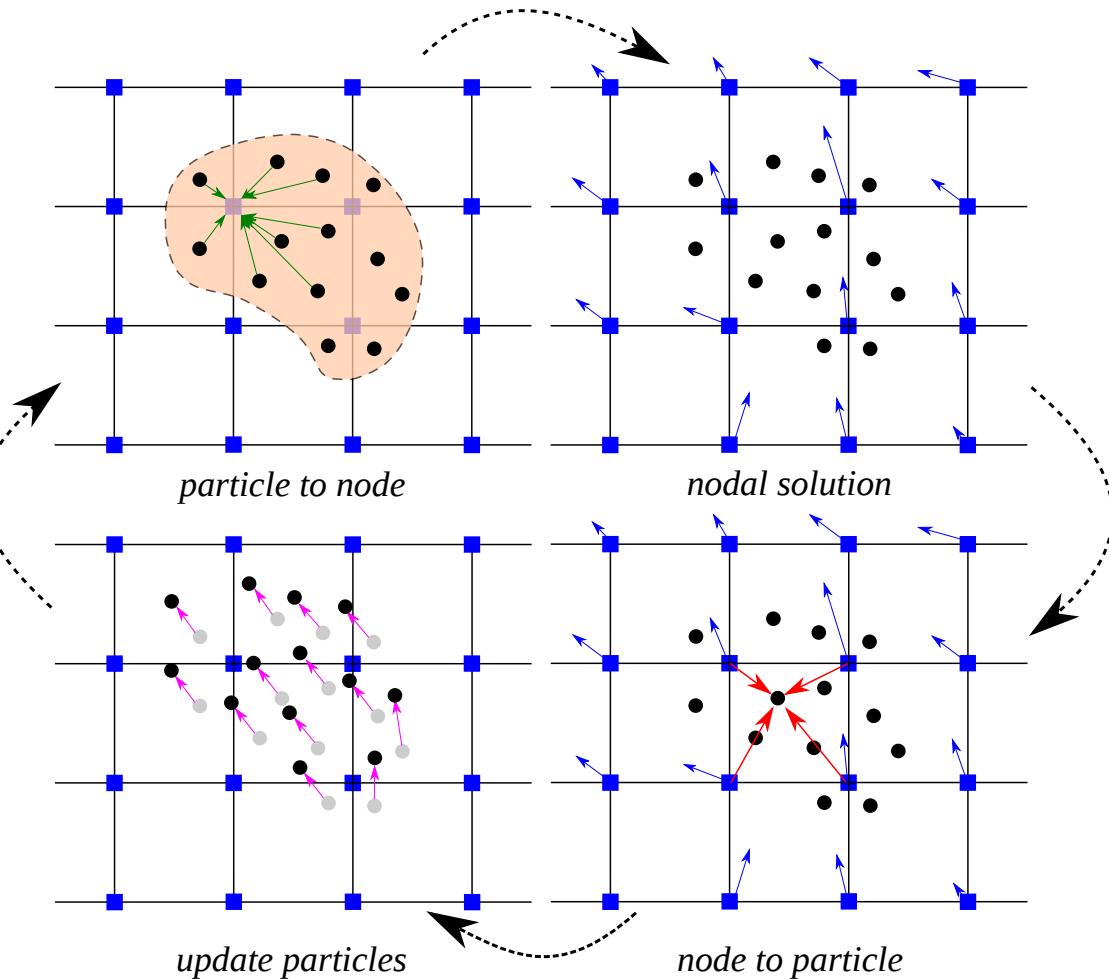


Figure 2.4 Illustration of MPM algorithm (1) A representation of material points overlaid on a computational grid. Arrows represent material point state vector (mass, volume, velocity, etc.) being projected to the nodes of the computational grid. (2) The equations of motion are solved on the nodes, resulting in updated nodal velocities and positions. (3) The updated nodal kinematics are interpolated back to the material points. (4) The state of the material points are updated and the computational grid is reset.

structure represented by the material points, and (2) understanding the qualitative trends associated with the material points like mass, velocity or stress.

The MPM output data contains both the material point and the grid data, and one approach in visualizing MPM data is by rendering the interpolated particle values on grid nodes using the *iso-surfacing* (Lorensen and Cline, 1987) or *volume rendering* (Levoy, 1988). In regions where the material points are sparse, it is necessary that the grid resolution is sufficiently fine to compensate for the missing features. This results in storing a large amount of unnecessary data in regions where sufficient material points are present. Thus, it is advantageous to visualize MPM data of the material points as particles (Bigler et al., 2006). Particle visualization involves rendering the particles as a sphere or an ellipsoid representing the size and location of the fraction of the continuum (Gumhold, 2003; Krogh et al., 1997; Kuester et al., 2001). In the present study, MPM data points are represented as spheres. Colour mapping of scalar quantities such as mass, velocity, or stress of a material point are applied to provide additional qualitative understanding of the data.

2.3.5 GIMP method

The shape functions used in MPM are continuous, and hence penetrations between bodies are handled automatically without the need for any supplemental contact algorithm (Chen and Brannon, 2002). In MPM, the continuum body deforms and moves in an arbitrary computation grid and all the boundary conditions are carried by the boundary particles. If a boundary particle is present in a cell, then the cell boundary becomes a part of the continuum body, and the cell size represents the thickness of the boundary. However, in certain cases both the boundary particle and an interior particle can be found in a cell, in which case the cell is still treated as a boundary cell, and the interior particle temporarily acts as a boundary particle. To avoid numerical errors, it is essential to use a smaller cell size along the boundary (Chen and Brannon, 2002).

In MPM simulations, numerical noise is observed when material points cross the cell boundaries as the body deforms, this is termed *cell crossing noise*. If a material point is located very close to the cell boundary, it results in discontinuous gradient of the weighing function causing a force imbalance on the grid (Bardenhagen and Kober, 2004). This results in large non-physical acceleration values resulting in separation of material points from the continuum (Sulsky et al., 1995). Figure 2.5 illustrates the problem of cell crossing noise. The main reason for the occurrence of cell crossing noise is the use of piecewise linear shape functions. However, this problem, which is predominant when using fine mesh size, can be overcome by changing the order of arithmetic operation as proposed by Sulsky et al. (1995).

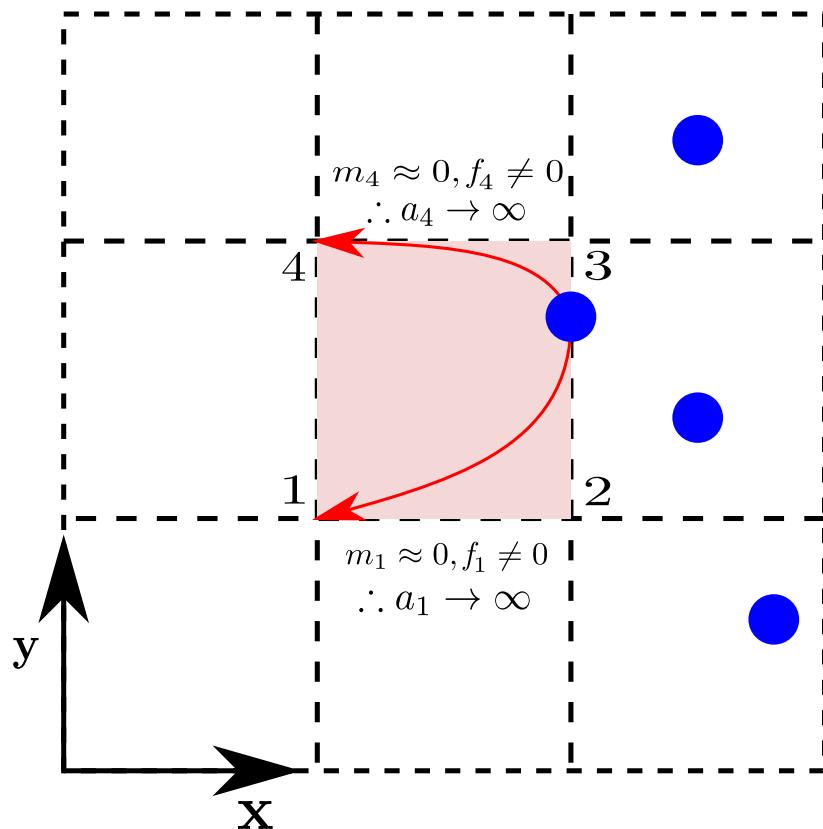


Figure 2.5 Schematic description of occurrence of cell crossing noise in MPM

To overcome the problem of cell crossing noise, Bardenhagen and Kober (2004) proposed an alternate method called the Generalized Interpolation Material Point Method that uses smoother shape functions and a larger influence region for each grid node. This approach minimizes the cell crossing noise. The piecewise-linear grid basis functions used are written as

$$\bar{\phi}(x) = \begin{cases} 1 - |x|/h & : |x| < h \\ 0 & : \text{otherwise}, \end{cases} \quad (2.25)$$

where h is the grid spacing. The basis function associated with grid node i at position x_i is then $\bar{\phi}_i = \bar{\phi}(x - x_i)$. The basis functions in 3-D are separable functions constructed as $\bar{\phi}_i(x) = \bar{\phi}_i^x(x)\bar{\phi}_i^y(y)\bar{\phi}_i^z(z)$. GIMP is often implemented using the standard piecewise-linear grid basis functions and piecewise-constant particle characteristic functions:

$$\chi_p = \begin{cases} 1 & : |x| < \frac{1}{2}l_p \\ 0 & : \text{otherwise}, \end{cases} \quad (2.26)$$

in which case the 1-D MPM and GIMP weighting functions can be grouped together in the general form

$$\bar{\phi} = \begin{cases} 1 - (4x^2 + l_p^2)/(4hl_p) & : |x| < \frac{l_p}{2} \\ 1 - |x|/h & : \frac{l_p}{2} \leq |x| < h - \frac{l_p}{2} \\ (h + \frac{l_p}{2} - |x|)^2/(2hl_p) & : h - \frac{l_p}{2} \leq |x| < h + \frac{l_p}{2} \\ 0 & : \text{otherwise}, \end{cases} \quad (2.27)$$

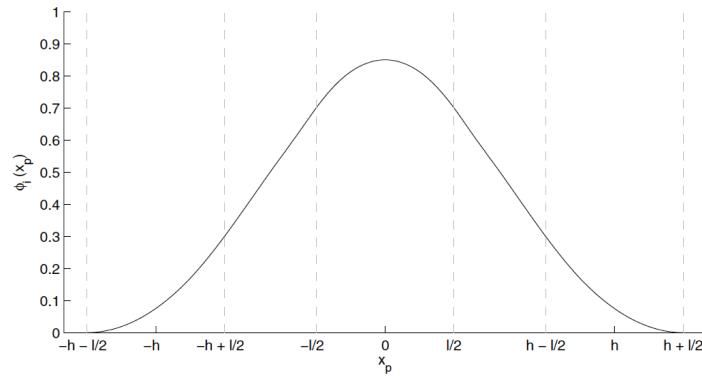
where l_p is the width of the particle characteristic function χ_p . figure 2.6a shows a 1-D GIMP weighting function $\bar{\phi}_{ip}$ and gradient weighting function $\nabla\bar{\phi}_{ip}$ for a piecewise-constant χ_p with a characteristic length of l . The GIMP weighting function is smooth, however a discontinuity is observed in the gradient weighting function.

In traditional MPM, boundary conditions only need be applied on those nodes which coincide with the extent of the computational domain. As illustrated in figure 2.6c nodes beyond those boundaries are not influenced by particles within the domain. This can be considered a result of the zero width of the Dirac delta characteristic functions. However, special attention is required to simulate the boundaries in the Generalized Interpolation Material Point Method (GIMP). Namely, because of their increased extents, it is possible for particles to influence, and be influenced by, nodes that lie outside of the simulation domain

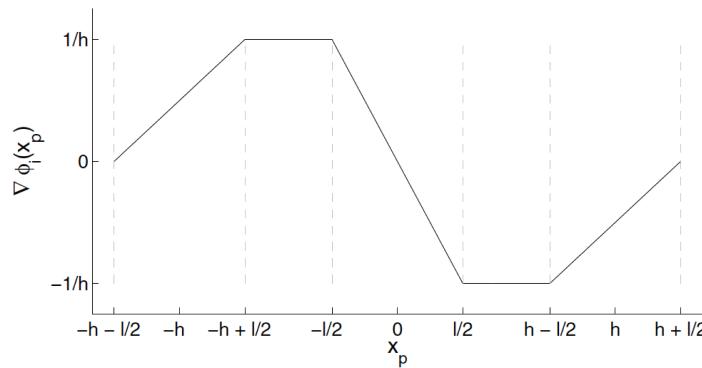
(figure 2.6b). These extra nodes are referred to as the “ghost” nodes. Boundary condition treatment of these nodes for Dirichlet conditions is the same as for the regular boundary nodes, namely, their computed values are replaced by prescribed values (Steffen et al., 2008).

In the present study, the influence of the GIMP method on the run-out behaviour of a granular column collapse experiment is investigated. Figure 1.7 shows a granular column of height H_0 and length L_0 is allowed to collapse and flow on a horizontal plane. The run-out distance observed is proportional to the initial aspect ratio of the column (H_0/L_0). A granular column with an initial aspect ratio of 0.4 is considered for the comparison. The granular column is represented by 32,000 material points arranged uniformly on a regular lattice with a particle spacing of 0.25 mm. Since, the scale of the problem being modelled is small and it is important to precisely define the flow surface, a larger number of material points are used to represent the geometry. However when modelling geophysical problems, where the tolerance in defining the flow surface is in the order of few millimetres, each material point shall represent individual grains or orders of magnitude larger than the grain size. A grid size of 1 mm is adopted with 16 material points per cell. In order to understand the influence of the number of material points on the accuracy of the solution, a simulation using 4 material points per cell with GIMP is also performed. The granular collapse experiment is performed for a column with an initial aspect ratio of 0.4 using both GIMP method and MPM with 16 material points per cell.

The evolution of run-out at time $t = \tau_c$ and $t = 6\tau_c$, where τ_c is the critical time when the potential energy is fully mobilised, are presented in figure 2.7. At the initial stage of collapse $t = \tau_c$, both MPM and GIMP give almost the same behaviour. The run-out observed in the case of 4 material points per cell is similar to the run-out behaviour for 16 material points per cell. At the end of the flow, the GIMP simulation with 4 material points show oscillations at the flow front due to fewer material points in a cell. However, both MPM and GIMP show a more smoother response at the flow front. The evolution of run-out and height with time for both MPM and GIMP are presented in figure 2.8. For a time up to $t = 1.5\tau_c$ all approaches yield the exact same behaviour. However, as the flow progresses, the number of material points per cell at the flow front decreases and this results in oscillations. The oscillations with decrease in the number of material points can be seen in the case of 4 material points per cell. Hence, it is essential to have a larger number of material points, especially at the flow front. The difference in the normalised run-out between MPM and GIMP method is about 2.5%. This is due to the difference in the interpolation scheme adopted in both approaches. GIMP method offers a better approximation of the run-out behaviour as a result of the continuous basis function. This also results in a more smooth stress and velocity distribution in GIMP than MPM. With increase in the number of material points and the

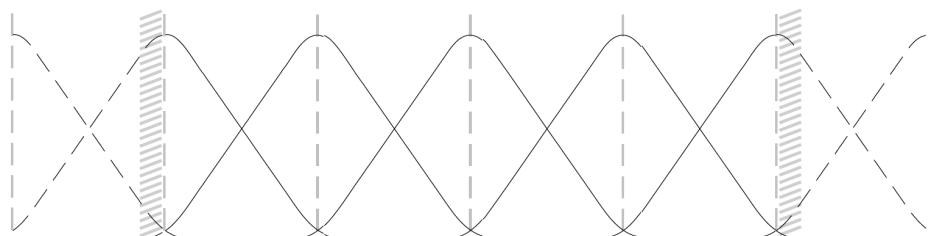


GIMP Weighting Function

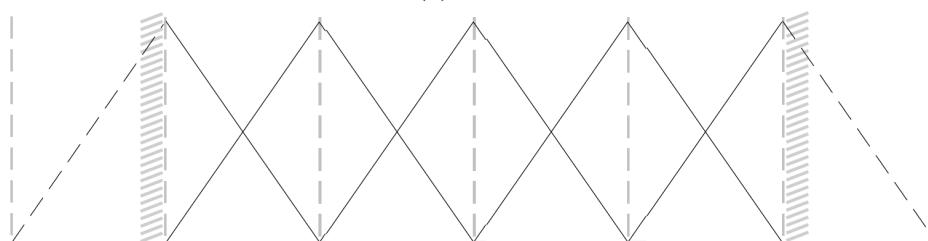


GIMP Gradient Weighting Function

(a) Example GIMP weighting function $\bar{\phi}_{ip}$, and gradient weighting function $\nabla \bar{\phi}_{ip}$ centered at 0 using piecewise linear grid basis functions and piecewise constant particle characteristic functions χ_p . Dotted lines denote breaks in the continuity of the functions.

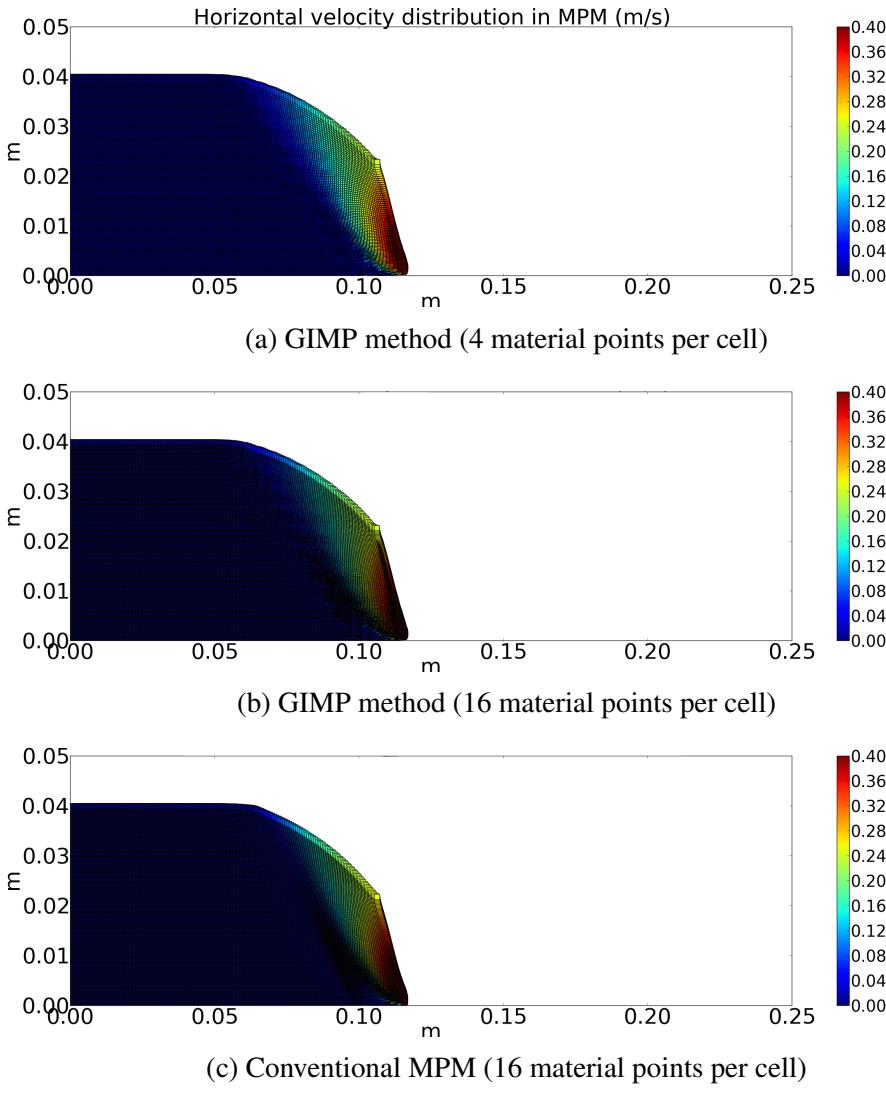


(b) GIMP



(c) Piecewise-Linear

Figure 2.6 Schematic view of 1-D basis functions used in MPM (Steffen et al., 2008).

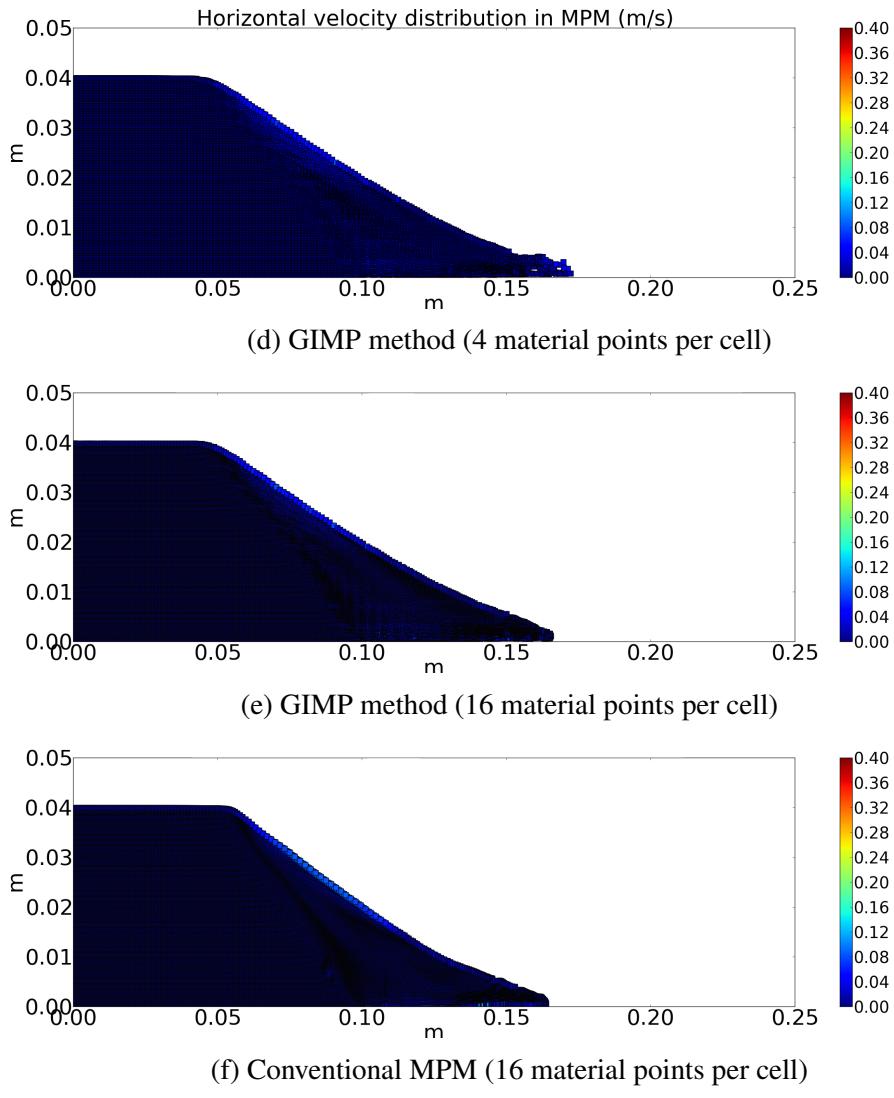


Evolution of granular column collapse at $t = \tau_c$.

use of finer mesh size decrease the difference between both approaches. The computational effort using GIMP method is almost twice that of MPM, since GIMP method considers the particles at neighbouring cells due to the larger spread of the basis functions. In the present study, a very fine mesh and 16 material points per cell are used to simulate large deformation problems.

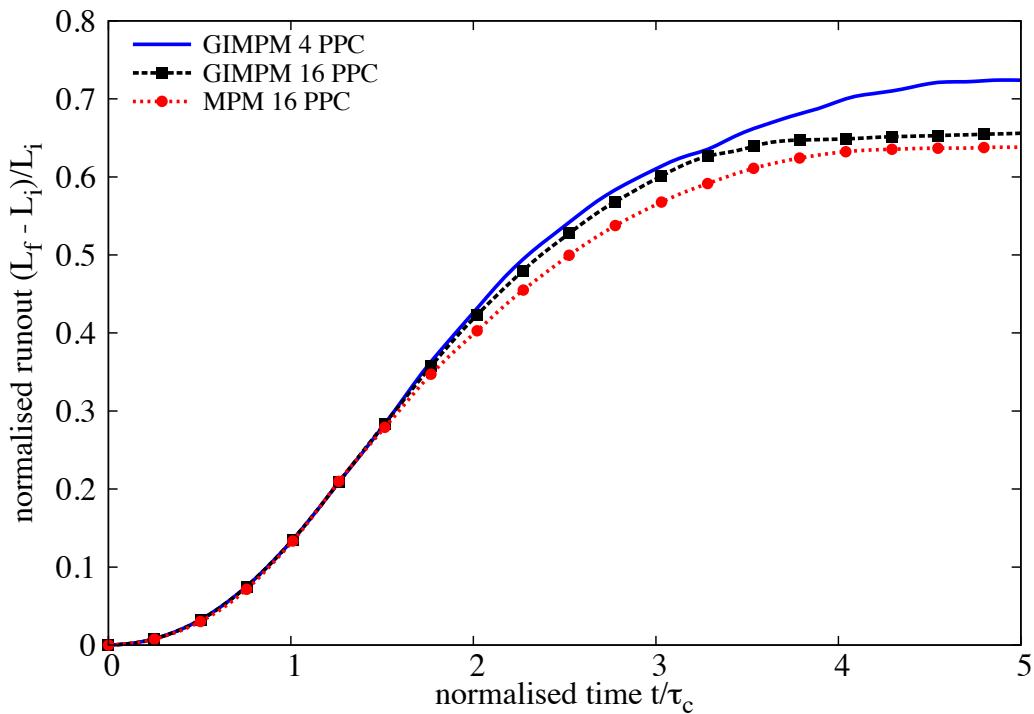
2.3.6 Application of MPM in geomechanics

The studies on using the material point method in modelling geotechnical problems are limited. The potential of the Material Point Method in modelling granular flows, due to the

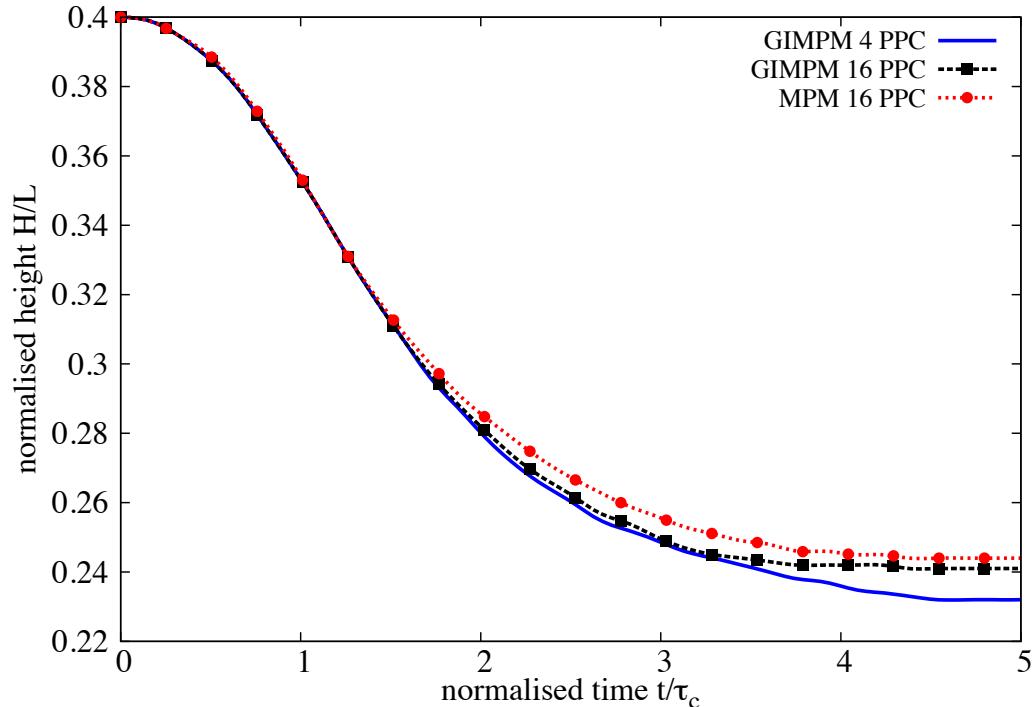


$$t = 6\tau_c$$

Figure 2.7 Comparison between GIMP method and conventional MPM on the flow morphology of a granular column collapse ($a = 0.4$).



(a) Evolution of run-out (GIMP method vs MPM)



(b) Evolution of height (GIMP method vs MPM)

Figure 2.8 Comparison between GIMP method and conventional MPM on the evolution of run-out and height with time for a granular column collapse ($a = 0.4$).

discharge of silos, was first recognised by Wieckowski et al. (1999). Bardenhagen et al. (2001) developed a frictional contact algorithm to model granular materials. The Mohr-Coloumb model criterion is used to describe the kinematics of the grains. In this model, a contact is defined when the nodal velocity interpolated from all material points in the cell differs from the nodal velocity interpolated from a single material point. Coetzee et al. (2005) applied this contact algorithm to understand the pull-out behaviour of anchors. Ma et al. (2014) developed a new contact algorithm with a penalty contact function and a limited maximum shear stress for soil-structure interaction, i.e, interaction of pipe-line with debris flow or submarine landslide. The penalty contact function behaves similar to numerical damping and thus reduces the oscillations during the impact.

Beuth et al. (2010) applied Gaussian integration in quasi-static MPM to model large strain problems. However in this approach, conservation of mass is not valid as a larger filled volume of material is considered. Andersen and Andersen (2010) used GIMP method with an elasto-plastic model to simulate slope failures. The solution is found to be dependant on the number of material points used to describe the slope geometry. Mast et al. (2014a) studied the behaviour of granular column collapse using a non-associative flow rule. They observed a significant increase in the run-out distance for large aspect ratio columns. Mast et al. (2014b) investigated the suitability of Material Point Method in the prediction of large deformation problems such as snow avalanches.

Guilkey et al. (2007) developed a coupled numerical scheme for fluid-structure interaction. The solid field is modelled in a Lagrangian frame, while an Eulerian frame, compressible CFD, is used for the fluid. As the MPM computation grid is reset at every stage, the same Eulerian grid is adopted for both the solid and the fluid. A similar approach was adopted by Zhang et al. (2008) to model multiphase flows, where the interactions between the solid and gas are modelled using the MPM background mesh as an Eulerian grid. Mackenzie-Helnwein et al. (2010) investigated various techniques to model multiphase drag forces. Both solid and fluid are modelled as Lagrangian particles using the mixture theory. Abe et al. (2013) developed a soil–pore fluid coupled MPM algorithm based on Biot’s mixture theory for solving hydro-mechanical interaction problems. Bandara (2013) developed a unique approach in modelling solid-fluid interactions. Two sets of Lagrangian particles are used to represent soil skeleton and pore water, separately. Bandara (2013) applied the coupled MPM to solve large deformation problems such as slope failure due to seepage.

In the present study, the Material Point Method is used to model large deformation problems, such as collapse of dry columns and soil slopes subjected to horizontal excitation. The suitability of the continuum approach (MPM) in modelling large deformation problems is also investigated.

2.4 Particulate modelling of granular flows

Granular materials often exhibit different behaviour under different circumstances. Fluidized granular material often resembles a liquid, and reveals surface waves. In certain situations, granular materials behave more like a solid exhibiting plastic deformations. Despite the wide variations in the physical and the chemical properties of the grains, the discrete granular structure has a rich generic phenomenology, which motivates us to understand the fundamental behaviour of these materials.

A granular material can be considered as a continuous material if it is viewed at a macroscopic scale, ignoring the fact that it is composed of grains. On a macroscopic scale, the behaviour of the granular material could be approximately defined using continuum mechanics. However, on a grain level, granular materials exhibit complex solid-like and/or fluid like behaviour depending on the way the grains interact with each other. Analytical and finite element models which consider granular materials as a continuum cannot take into account the local geometrical processes that govern the mechanical behaviour of a non-homogeneous soil. The application of continuum models to describe granular flow poses subtle problems for statistical analysis (Mehta and Barker, 1994). The grain level description of the granular material enriches the macro-scale variables, which poorly account for the local rheology of the materials.

Numerical models such as the Discrete Element approach proposed by Cundall and Strack (1979) are capable of simulating the granular material as a discontinuous system. Although, modern measurement techniques can probe into local granular variables, like grain position, velocities, contact forces, etc., they have inherent limitations in acquiring those variables. The *discrete-element* approach is a powerful and a reliable research tool to study the behaviour of granular materials at the grain-scale. This approach involves applying Newton's equation of motion simultaneously to all grains described as rigid solid bodies by considering the contact forces and the external forces acting on the grains. For a given boundary condition, the collective mechanical response of grains to the external force leads to relative motion between grains constrained in a dense state and/or by inelastic collisions in the loose state. Cundall and Strack (1979) applied this method to granular geomaterials, and called it the *Distinct Element Method*, to differentiate from the existing *Finite Element Method* used in geomechanics. The attribute "distinct" refers to the degrees of freedom of individual grains, but it was later replaced by "discrete" to underline the discrete nature of the system.

The interactions between the individual grains are governed by unilateral contact laws, and the mechanism of energy dissipation is through friction and inelastic collisions. Moreover, granular materials have a wide variation in their grain shape and size distribution that require

appropriate numerical treatments. In DEM, the normal reaction force, which prevents the interpenetration of two grains is proportional to the depth of penetration. Thus, frictional contact between grains can be expressed as a function of the configuration variables, which describe the positions and velocities of the grains (Radjai and Dubois, 2011).

Discrete-Element methods, which describe interactions between grains based on the explicit overlap between the grains are termed as *smooth methods*. Another approach is the *non-smooth approach* (Jean, 1999), which describes the behaviour of discrete elements using the main features of uni-laterality and Coulomb friction, and by neglecting the finer details such as interpenetration and overlap between grains. The fundamental difference between the non-smooth method and the common discrete element method lies in the treatment of small length and time scales involved in the dynamics of granular media. In DEM, the grains are treated as rigid bodies but the contacts between grains are assumed to obey the visco-elastic constitutive law. The time-stepping schemes used for the numerical integration of the equations of motion in DEM, imply that the contact interactions involve smaller time and length scales. In the non-smooth Contact Dynamics (CD) method, these small scales are neglected and their effects are absorbed into the contact laws. In non-smooth formulation, the grain dynamics is described at a larger scale than the elastic response time and displacement scales (Jean, 1999; Radjai and Richefeu, 2009).

DEM simulations can easily capture the complex flow mechanics of large-deformation problems than the continuum approach. Tang et al. (2009) used 2D discrete element modelling to understand the mechanism of the Tsaoling landslide triggered by the Chi-Chi earthquake. The authors were able to establish the landslide characteristics to have a low-friction coefficient (about 0.15) and a medium strength. They were also able to back-calculate a maximum velocity of sliding reached 50 m/s. Similarly, Tang et al. (2013) performed 3D discrete-element simulations to understand the transportation and deposition of the 2009 Hsiaolin landslide. The authors estimated the friction coefficient of landslide-mass to have reached a critical value of 0.1, at which the mass begins to slide and reach a maximum velocity of 40 - 50 m/s. Two-dimensional DEM simulations have been used to analyse the temporal and spatial evolution of slope failure and landslides from the intact, pre-failure slope to the stabilised, post-failure slope composed of bonded material (Katz et al., 2014). The pre-failure slope material disintegration is found to be the fundamental element in determining the size and geometry of the resultant landslides. Liu and Koyi (2013) studied the kinematics and internal deformation of granular slopes which experience flow-like behaviour. They observed dilatant grain-shearing flow is the dominating mechanism in the movement of granular slopes. DEM is capable of probing the material response in a detailed scale, where conventional experiments or field tests are not feasible. Hence, in the present study, 2D discrete element

simulations are performed to understand the behaviour of granular flows. Rickenmann et al. (2006) applied 2D debris-flow simulation models to two well-documented field events. Two-dimensional simulations provided reasonable results for the extent of deposits and the relative spatial distribution of deposit thicknesses. Nevertheless, some general characteristics of debris flow deposits, which are necessary for hazard assessment, may be reasonably well simulated with these simple modelling approaches if rheologic or friction parameters can be measured or calibrated.

2.5 Discrete Element Method

The Discrete Element Method (DEM) computes the equilibrium and the trajectories of a classical multi-body system. The Discrete Element Method is a simple and flexible discrete-element approach, which involves applying Newton's second law of motion to each grain to describe the deformation of the granular assembly.

$$m_i \frac{d^2 \mathbf{x}_i}{dt^2} = \mathbf{F}_i, (i = 1, \dots, N), \quad (2.28)$$

where N is the number of grains in the simulation, m_i is the mass of a grain i , \mathbf{x}_i is its position, and \mathbf{F}_i is the force exerted on grain. The method consists of calculating the forces \mathbf{F}_i and then solving the ordinary differential in eq. 2.28. In general the system of coupled non-linear differential equations cannot be solved analytically. The approximate numerical solution of these equations, which describes the trajectories of all the grains of the system is called as the Discrete Element Method.

DEM simulates similar to the real experiments, involving the generation of samples (initial conditions) with N grains and solving the Newton's equation of motion for the system until the properties of the system no longer change with time (equilibration of the system). The computation of the forces and torques is the central part of the Discrete Element Method simulation. The dynamics of the granular material is governed by Newton's equation of motion which depends on the centre-of-mass coordinates and the Euler angles of the grains i ($i = 1, 2, \dots, N$):

$$\frac{\partial^2 \vec{r}_i}{\partial t^2} = \frac{1}{m_i} \vec{\mathbf{F}}_i(\vec{r}_j, \vec{v}_j, \vec{\varphi}_j, \vec{\omega}_j), \quad (2.29)$$

$$\frac{\partial^2 \vec{\varphi}_i}{\partial t^2} = \frac{1}{\hat{J}_i} \vec{\mathbf{M}}_i(\vec{r}_j, \vec{v}_j, \vec{\varphi}_j, \vec{\omega}_j), (j = 1, \dots, N). \quad (2.30)$$

The force $\vec{\mathbf{F}}_i$ and the torque $\vec{\mathbf{M}}_i$, which act on grain i of mass m_i and the tensorial moment of inertia \hat{J}_i are (sometimes complicated) functions of the grain positions \vec{r}_j , their angular orientations $\vec{\phi}_j$, and their corresponding velocities \vec{v}_j and $\vec{\omega}_j$. In a two-dimensional system, the angular orientation of a grain is described by a single (scalar) quantity ϕ_i and the moment of inertia reduces to a scalar value J_i .

For grains in the absence of long range fields, the force $\vec{\mathbf{F}}_i$ and the torque $\vec{\mathbf{M}}_i$ acting upon the grain i are given as sum of the pairwise interaction of grain i with all other grains in the system:

$$\vec{\mathbf{F}}_i = \sum_{j=1, j \neq i}^N \vec{\mathbf{F}}_{ij}, \quad \vec{\mathbf{M}}_i = \sum_{j=1, j \neq i}^N \vec{\mathbf{M}}_{ij}. \quad (2.31)$$

The limitation to pairwise interaction is an abstraction, which is justified if the grain deformation at the contact is trivial. To describe the deformation of granular assemblies one has to take into account the effect of multi-grain interactions. This method is general and can be applied to a wide range of systems. The Discrete Element Method can be used to study the behaviour of grains in rapid flows and in static assemblies. The method treats both conditions in exactly the same way, it is not necessary to divide the system and then treat each condition differently. The simplest model for a grain is a sphere. In a two-dimensional case, the sphere is reduced to a circular disk. Simulations using spherical grains are numerically very effective since grain collisions can be easily identified and described in a simple way (Poschel and Schwager, 2005).

In the present study, a two-dimensional DEM code is developed in C++ to study the micro-scale rheology of dry granular flows. Existing DEM codes do not yet fully support micro-scale fluid solid coupling using Lattice Boltzmann approach, which will be used to study the mechanism of submarine landslides. A new C++ based high performance DEM code is developed in the present study. The features implemented in the present study and the general overview of DEM are discussed below.

2.5.1 The Forces

The force \mathbf{F}_i in eq. 2.28 represents both the grain to grain interaction force, and other external forces acting on the system. Therefore, the force \mathbf{F}_i is expressed as

$$\mathbf{F}_i = \sum_{j \neq i} \mathbf{F}_{ij} + \mathbf{F}_{ext,i}, \quad (2.32)$$

where \mathbf{F}_i is the force exerted by grain j on i . The external force $\mathbf{F}_{ext,i}$ is most often the force of gravity, $\mathbf{F}_{ext,i} = m_i \mathbf{g}_i$. The methodology to incorporate any other external forces in the simulation is the same. However, the computation of the interaction forces depends on the numerical method adopted in the study. The methodology used in the present study is described below.

Let us consider two grains i and j , in contact (figure 2.9). The contact force can be decomposed into two components, as the normal (F_n) and the tangential (F_t) components

$$\mathbf{F}_{ij} = F_n \mathbf{n} + F_t \mathbf{t}. \quad (2.33)$$

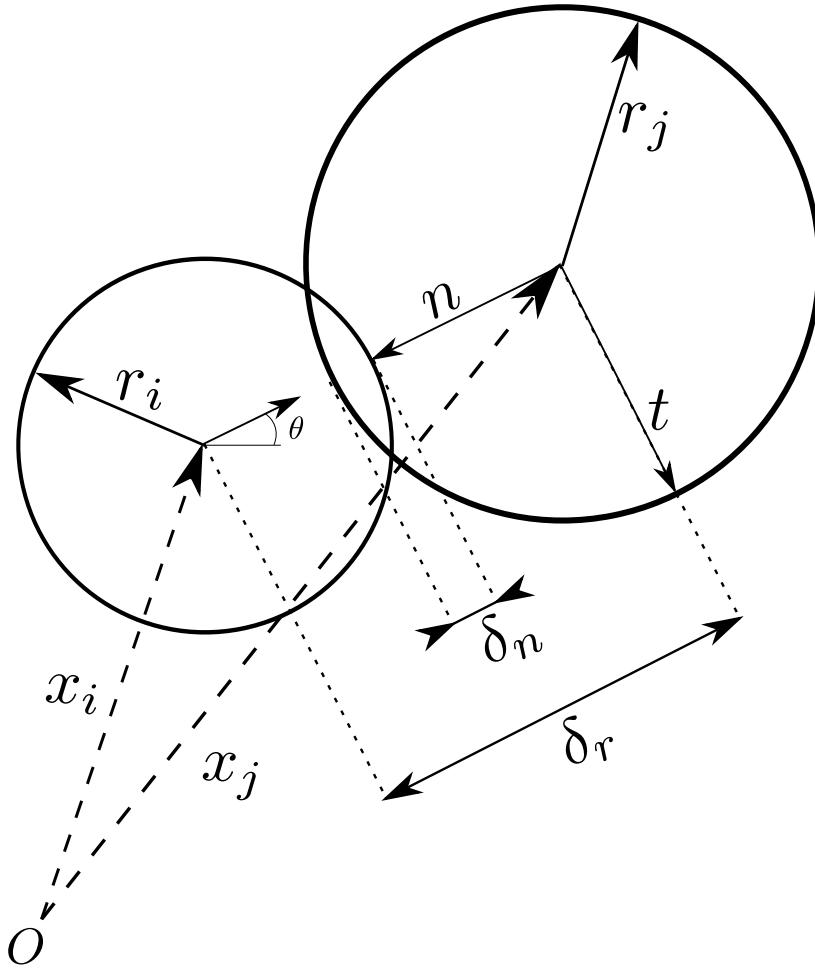


Figure 2.9 Grains i and j in contact, and the separation δ_n is used to calculate the normal force

where \mathbf{n} and \mathbf{t} are unit vectors, pointing in the normal and the tangential directions. The procedure adopted to calculate the normal and tangential forces are discussed.

Normal force

When grains collide, part of the kinetic energy is dissipated as heat and the other part causes deformation of the grain. These deformations generate interaction forces. In DEM, the grains are considered to be rigid while their contact is assumed to be soft. Thus, the grains do not change their shape, instead they overlap. The shapes of the grains are conserved on an average, after many collisions. The overlap at the contact is limited to very small deformations, which are achieved by defining a repulsive normal force that opposes the overlap. The mutual compression (δ_n) of the grains i and j is defined as

$$\delta_n = |x_i - x_j| - r_i - r_j, \quad (2.34)$$

where x_i and x_j are vectors fixing the centres of the grains and r_i and r_j are their radii (figure 2.9). When $\delta_n > 0$, the two grains are not in contact, and there is no interaction. When $\delta_n < 0$, the two grains overlap, and there is a repulsive normal force that pushes the two grains apart. The simplest model is to consider the contact as a linear spring with damping. The repulsive force depends linearly on δ_n , and is controlled by the stiffness of the grain. The energy dissipation due to the interaction between grains is an intrinsic characteristic of the granular material and is incorporated by adding a damping force that opposes the relative velocity for the duration of the contact. The interaction force at the contact is idealized as a simple spring-dashpot system, with elastic and dissipative constants (Luding et al., 1994).

$$F_n = \begin{cases} 0, & \delta_n > 0 \\ -k_n \delta_n - \gamma_n \frac{d\delta_n}{dt}, & \delta_n < 0 \end{cases} \quad (2.35)$$

The constant k_n characterises the stiffness of the grain, and must be chosen to be sufficiently large that the overlap between the grains remain small. Nevertheless, the solution has an undesirable property of generating an attractive force (Poschel and Schwager, 2005). It arises just before the two grains separate. In this case, we have $d\delta_n/dt > 0$ while δ_n approaches zero. To avoid the attractive force, the force is computed in two stages: a candidate force \hat{F}_n is calculated, and verified whether it is non-negative

$$\hat{F}_n = -k_n \delta_n - \gamma_n \frac{d\delta_n}{dt}, \quad F_n = \begin{cases} 0, & \hat{F} \leq 0 \\ \hat{F}_n, & \hat{F} > 0 \end{cases} \quad (2.36)$$

For pairwise collisions, the normal force (F_n) represented as $k_n \delta_n + \gamma_n$ causes a decrease in the relative normal velocity of the grains by a factor ε . This factor is the *coefficient of*

restitution, and is defined as $\varepsilon \approx u'/u$, where u is the absolute normal relative velocity before the collision and u' corresponds to the post-collision value. The relative velocity, $d\delta_n/dt > 0$, can be obtained by differentiating eq. 2.34. Thus we obtain

$$\frac{d\delta_n}{dt} = (\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}, \quad (2.37)$$

where $\mathbf{v}_i = dx_i/dt$ is the velocity of grain i and $\mathbf{v}_j = dx_j/dt$ is the velocity of grain j . The numerical integration of eq. 2.37 yields the separation δ_n and permits us to generalise the model and treat the tangential forces as well, as explained in the next section. By integrating Newton's equation of motion it is found that the linear force corresponds to the co-efficient of restitution, which is defined as

$$\varepsilon = \exp\left(-\frac{\pi\gamma_n}{2m^{eff}}/\sqrt{\frac{Y}{m^{eff}} - \frac{\gamma^n}{2m^{eff}}^2}\right). \quad (2.38)$$

Tangential force

Grains are not perfect spheres, but have a complicated surface texture. Therefore, at oblique collisions, besides the normal force there is a tangential force too. Even perfectly smooth spheres exert a tangential force due to their bulk viscosity (Poschel and Schwager, 2005). To build a heap of spheres on a flat surface, the grains as well as the surface have to be sufficiently rough, indicating the dependence of the tangential force on the surface properties of the granular materials. For realistic simulation of granular materials, it is important to consider the tangential force in DEM. The tangential force is considered in a similar fashion as the normal force, arising from a spring stretched by the relative motion of the grain. Tangential forces are modelled by considering the relevant relative tangential velocity of the grain surfaces at the point of contact. The point of contact is an approximation, as the description of the normal force assumes a compression δ_n , which implies a contact surface in 3-D or a contact line in 2-D. Assuming a tangential spring of length δ_t exerts an opposing force to the relative tangential displacements (ignoring the effect of relative rolling between the grains), the tangential force can be postulated similar to the normal force (eq. 2.37) as

$$\frac{d\delta_t}{dt} = (\mathbf{v}_i - \mathbf{v}_j) \times \mathbf{t}. \quad (2.39)$$

This equation must also be numerically integrated, just like eq. 2.28. The grains are in contact when $\delta_t < 0$ and when $\delta_t = 0$, the grains no longer exert a force on each other. With these assumptions, δ_t can be calculated similar to the normal force. The tangential force is assumed

to be governed by Coulomb's friction law.

$$|F_t| \leq \mu F_n, \quad (2.40)$$

where F_t is the tangential force and μ is the friction coefficient. It is therefore necessary to constrain the tangential force to remain less than or equal to μF_N . To impose the condition in eq. 2.40, two-stages similar to the normal force computation is adopted. The first step is to evaluate the candidate force, and is then accepted if it obeys the condition in eq. 2.40.

$$\hat{F}_t = -k_t \delta_t - \gamma_t \frac{d\delta_t}{dt}, \quad F_t = \begin{cases} sgn(F_t), & |\hat{F}| \geq \mu F_n \\ \hat{F}_t, & |\hat{F}| < \mu F_n \end{cases} \quad (2.41)$$

where k_t is the stiffness of the tangential spring and γ_t is the damping constant. If $|F_t| = \mu F_n$, the contact is sliding, otherwise, it is non-sliding. It can be noted that the normal force (eq. 2.36) and the tangential force (eq. 2.41) are handled in the same way in DEM. When the grains slide against each other, they do not retain any memory of their initial position, and hence do not return to its original position. In order to model this behaviour, a limiting value of δ_t is imposed. When the contact slides $\delta_t = \pm \mu F_n / k_t$ is imposed.

In addition to sliding, the grains can roll relative to one another about their centre of mass due to the tangential force acting at their contact surface. In this case, $d\delta_t/dt = 0$. It is important to assume that the grains touch at a single point instead of overlapping, i.e. $\delta_n = 0$. This point is located at $x_i - r_i \mathbf{n} = x_j + r_j \mathbf{n}$. If we consider that this point belongs to grain i , its velocity is $v_i + r_i(\boldsymbol{\omega} \times \mathbf{n})$. If it belongs to grain j , its velocity is $v_j + r_j(\boldsymbol{\omega} \times \mathbf{n})$. The relative velocity is the difference between these two velocities.

$$\frac{d\delta_t}{dt} = (\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{t} - (r_i \boldsymbol{\omega}_i + r_j \boldsymbol{\omega}_j) \times \mathbf{n}. \quad (2.42)$$

It should be noted that the eq. 2.42 is only an approximation, as the grains in DEM do not touch at points, but overlap. It is therefore an approximation that produces an error of order $O(\delta_n/r)$ (Radjai and Dubois, 2011). It is assumed that the contact forces are exerted at the point of contact. It implies that the tangential force is accompanied by torque acting on two grains. If the overlap is zero, these torques are

$$\tau_{ij} = -(a_i \mathbf{n}) \times (F_t \mathbf{t}), \quad (2.43)$$

$$\tau_{ji} = -(a_j \mathbf{n}) \times (F_t \mathbf{t}). \quad (2.44)$$

The torques modify the angular velocities of the grains. It is therefore necessary to incorporate the equation for the angular coordinates of the grains in eq. 2.28

$$I_j \frac{d\omega_i}{dt} = \sum_{j \neq i} \tau_{ij}, \quad (2.45)$$

where I_j is the moment of inertia of grain j . Eq 2.44 is only valid when $\delta_n = 0$. The torque is a vector product of the force and its lever arm. It is assumed that the lever arms have lengths equal to r_i and r_j , which is true only when the grains do not overlap, hence in this case they produce an error of order $O(\delta_n/r)$. It is nevertheless desirable to damp this type of motion (Radjai and Dubois, 2011). A rolling resistance can be adopted in order to model the shape effect of non-spherical grains, which accounts for moments arising from the fact that the line of action of the normal contact force in the case of non-spherical particles no longer passes through the centre of mass of the particles and hence generates rotational moments.

The interaction between two solid bodies is much more complex than that is described by the simple linear model. Nevertheless, the linear force law has several advantages. It is simple to implement, and its harmonic behaviour is well understood, which makes it easier to interpret the results. The most common non-linear interaction law is the Hertz law (Hertz, 1882). In certain situations, such as a quasi-static packing, a non-linear law can have significant influence on the acoustic properties, and on the global stiffness (Agnolin and Roux, 2007). However, in case of rapid granular flows, the interaction force between the grains has almost no effect on the phenomenon, and a linear law can be used to describe this kind of behaviour (Radjai and Dubois, 2011).

2.5.2 Numerical algorithm and integration scheme

The efficiency of a DEM algorithm is mainly determined by its efficiency to compute the interaction forces between grains. If we consider a model system with pairwise interactions, we have to consider the contribution of the force on grain i due to all its neighbours. If we consider only the interaction between a grain and the nearest image of another grain, then for a system of N grains, we must evaluate $N \times (N - 1)/2$ pair distances. Consider a system of 1000 grains, at every time step all possible pairs of grains have to be considered to compute the interaction forces, hence, $N(N - 1)/2 \approx 500,000$ force computations are required. For short-range grain interactions, the majority of these force evaluations is unnecessary as the corresponding grains are located far apart and do not necessarily touch each other. For a dense system of equally sized grains, the grains can have contacts with not more than 6 grains, this reduces the number of force computation required to $3N \approx 3000$.

In the preliminary force computation scheme, at least 166 times more pair interactions are considered than necessary. Therefore, the numerical methods employed in the DEM should try to minimize the computation of interaction forces (Poschel and Schwager, 2005). There are three different methods for the efficient computation of the forces, the *Verlet* algorithm, the *link-cell* algorithm, and a *lattice* algorithm. The *Verlet* algorithm described in Grubmuller et al. (1991) is implemented in the present study.

Verlet list algorithm

The Verlet list algorithm assumes a cut-off value, so that only neighbouring grains that contribute to the energy of a grain i are considered. It is advantageous to exclude the grains that do not interact in the memory expensive energy computation. Verlet (1967) developed a book-keeping technique, commonly referred to as the Verlet list or neighbour list, which is illustrated in 2.10. In this method a second cut-off radius $r_v > r_c$ is introduced, and before the interactions are calculated, a list is made (the Verlet list) of all grains within a radius r_v of the grain i . In the subsequent calculations of the interactions, only those grains in this list will be considered. The idea of the Verlet algorithm is based on a simple property of grain dynamics: the neighbourhood relation between grains can only change slowly, i.e. two grains which are close to each other at a given time step will remain as neighbours, at least in the following few time steps. During initialization the neighbourhood relations between the grains, i.e. the distance of all close pairs of grains are computed. Two grains are considered as neighbours if the distance of their surface is smaller than a predefined distance *Verlet distance*

$$(|\vec{r}_i - \vec{r}_j| - R_i - R_j) < \text{Verlet distance}. \quad (2.46)$$

For each grain there is a *Verlet list* in which the close neighbours are saved. To initialise the Verlet lists efficiently, a grid that covers the simulation area is defined. Its mesh size is larger than the largest grain. For construction of the lists only pairs whose grains reside in the same or adjacent grids are considered. This procedure guarantees the detection of all close pairs of grains (Poschel and Schwager, 2005). Redundancy in Verlet lists, i.e. if grain i is a neighbour of j , then grain j is a neighbour of i , are avoided by imposing a restriction on the list of grain i contains, such that it contains only neighbours with index $j < i$. For the computation of interaction forces, the Verlet list of grain i is scanned and only pairs which are recorded in one of the Verlet lists are considered. Hence, the Verlet list of each grain i is scanned and the interaction force of i with each entry j in its list is computed.

Initially to build the Verlet list, the grains are sorted into a grid of mesh size $dx \times dy$. For each grid there is a list of grains residing in the cell. During the simulation, the neighbourhood

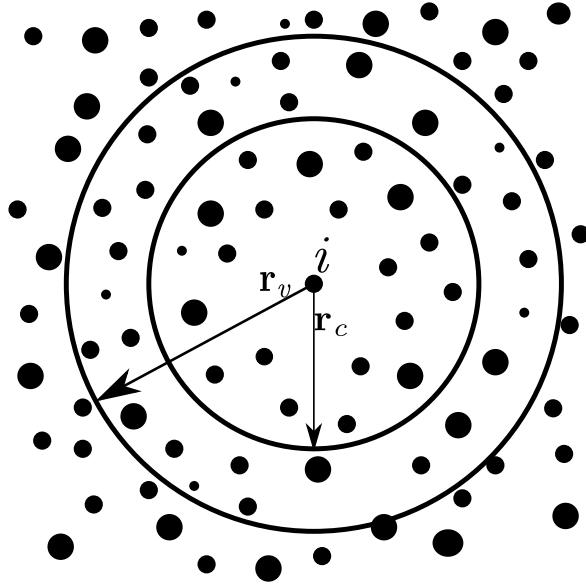


Figure 2.10 The Verlet list: a grain i interacts with those grains with the cut-off radius r_c , the Verlet list contains all the grains within a sphere with radius $r_{v>r_c}$

relation among the grains change, therefore, the Verlet lists have to be updated. The decision to update a Verlet list depends on how far the grains have travelled since the time when the present list was built. The Verlet list of a grain i must contain at any time all neighbours j with $j < i$. This assures that two grains i and j never touch and are not considered as neighbours, i.e. j is not in the list of i and i is not in the list of j . Hence,

$$|\vec{r}_i - \vec{r}_j| - R_i - R_j > 0. \quad (2.47)$$

The above condition is required for all pairs (i,j) of grains which are *not* known as neighbours. This condition is a criterion to update the Verlet lists (Poschel and Schwager, 2005). Assume at the instant when the Verlet lists are constructed, the surfaces of the grains have the distance $|\vec{r}_i - \vec{r}_j| - R_i - R_j >$ Verlet distance, i.e. they are not classified as neighbours. If the Verlet lists are updated before one of these grains has travelled the distance $\text{verletdistance}/2$ since the lists were constructed, they can never collide without being recognized as neighbours first. This is explained in figure 2.11. The impact of optimisation of the Verlet list algorithm has negligible effect on the computation time, as the algorithm is quite efficient already and only consumes a few percent of the total computation time in construction of the Verlet lists. The implementation of the Verlet list algorithm in force computation drastically reduces the computation time in comparison to the linear algorithm. The performance of the Verlet list algorithm is controlled by two crucial parameters: the

number of cells N_c , for the construction of the Verlet lists and the Verlet distance r_v (Poschel and Schwager, 2005).

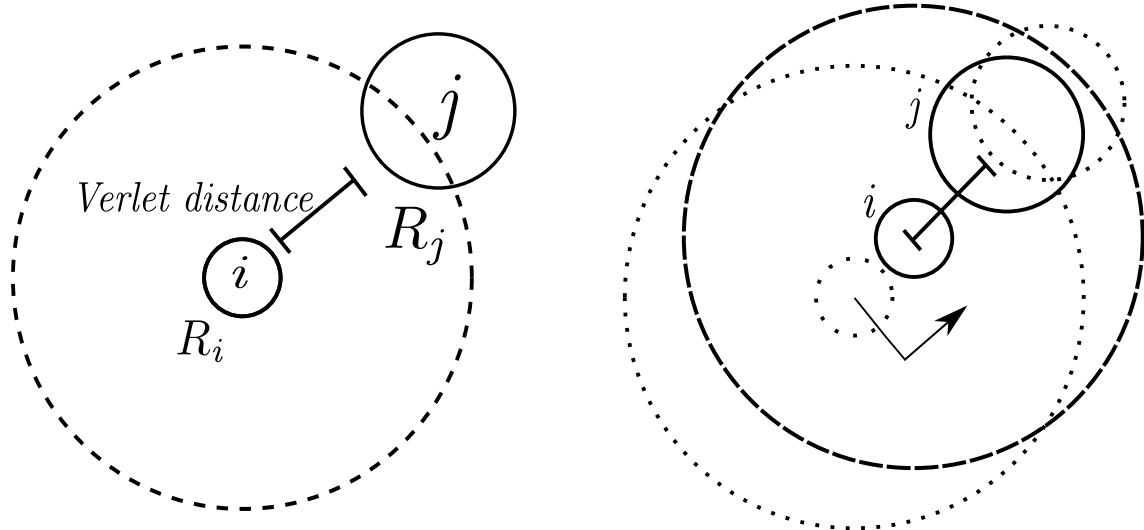


Figure 2.11 Checking the validity of Verlet lists. *Left:* the grains i and j are not recognized as neighbours since the distance of their surface is larger than the Verlet distance. The radius of the dashed circle is $R_i + R_{max} + \text{Verlet distance}$. *Right:* in the most unfortunate case the grains approach each other directly, travelling at the same velocity. As soon as one of the grains has travelled the distance $\text{Verlet distance}/2$ (arrows), the Verlet lists have to be rebuilt. The grains i and j are now recognized as neighbours. Redrawn after Poschel and Schwager (2005).

Leap frog or Verlet integration algorithm

Discrete Element Method involves numerically solving Newton's equation of motion eq. 2.28, which is an ordinary differential equation. Choosing an integration algorithm is important, as the forces are not always differentiable in time, and the temporary derivative of the force is discontinuous when the contact splits. It is also very essential to numerically integrate eq. 2.42 with the same precision as eq. 2.28. At first, computational speed seems important. It is usually not very relevant because the fraction of time spent on integrating the equation of motions (as opposed to computing the interactions) is small. Accuracy for large time steps is more important, because the larger the time step that we can use, the fewer evaluation of the forces are needed per unit of simulation time. Hence, this would suggest that it is advantageous to use a sophisticated algorithm that allows use of larger time step.

Algorithms that allow the use of large time steps, achieve this by storing information on increasingly higher-order derivatives of the grain coordinates. Consequently, they tend to require more memory storage. However, the most important aspect to consider is the energy conservation. It is important to distinguish between two kinds of energy conservation: the

short time and long time. The sophisticated higher-order algorithms tend to have very good energy conservation at short times. However, they often have undesirable feature that results in drifting of the overall energy for longer times. In contrast, the Verlet style algorithms tend to have only moderate short term energy conservation, but little long-term drift (Frenkel and Smit, 1996). In this case, such algorithms are not useful. They are more complicated to program, and do not yield a more precise solution (Radjai and Dubois, 2011). It might seem important to have an algorithm that accurately predicts the trajectories of all grains for both short and long durations, however no such algorithm exists.

In certain cases, two trajectories that are initially very close may diverge exponentially as time progresses. Any integration error, however small it may be, would always diverge the predicted trajectory exponentially from the true trajectory. This phenomenon is called the Lyapunov instability, and it poses a serious threat to the whole idea of Discrete Element Method simulation. However, this problem might not be serious (Frenkel and Smit, 1996). The aim of DEM is not to predict precisely what will happen to a system, but to predict the average behaviour of the system that is prepared in an initial state about which we know something (initial position, velocity and energy), but not everything. Hence, DEM differs from other methods, which are used to predict the trajectories. However, considerable numerical evidence suggest that the shadow orbits exists, which is a true trajectory of a multi-body system that closely follows the numerical trajectory for a time that is longer in comparison with the time that is required for the Lyapunov instability to develop (Frenkel and Smit, 1996).

Newton's equations of motion are time reversible, and so should be the integration algorithm. The "leapfrog" algorithm or the Verlet integration algorithm is a numerical scheme used to integrate the Newton's equation of motion to calculate the trajectories of grains and is implemented in DEM by Verlet (1967). The Verlet algorithm is fast and requires less storage memory, it is not particularly accurate for long time steps, and hence, we should expect to compute the forces on all grains rather frequently. Its short-term energy conservation is fair (in versions that use more accurate expression for velocity), but most importantly it exhibits little long-term energy drifts. This is related to the fact that the Verlet algorithm is time reversible and area preserving, however, it does not conserve the total energy of the system exactly (Frenkel and Smit, 1996). The Verlet algorithm is simply based on a truncated Taylor expansion of grain co-ordinates.

$$t(t + \Delta t) = rt + \mathbf{v}(t)\Delta t + \frac{f(t)}{2m}\Delta t^2 + \dots \quad (2.48)$$

If we truncate this expansion beyond the term Δt^2 , we obtain Euler's algorithm, which looks similar to the Verlet Algorithm, but it does not preserve energy and has significant energy drifts. The simplest among the Verlet schemes is the *Leap frog algorithm*, which evaluates the velocities at half-integer time steps and uses these velocities to compute the new positions. The position of each grain is calculated at time $t = 0, \Delta t, 2\Delta t, \dots$, where Δt is the time step. On the other hand, their velocities are calculated at intermediate times, that is, at $t = \Delta t/2, 3\Delta t/2, \dots$. Let the position of a grain at time $t = k\Delta t$ be written as x_k , and its velocity at time $t = \Delta t(k + 1/2)$ be written $\mathbf{v}_{k+1/2}$, and its acceleration at $t = k\Delta t$ be \mathbf{a}_k . Then the following equation is used to advance systematically

$$\mathbf{v}_{k+1/2} = \mathbf{v}_{k-1/2} + \mathbf{a}_k \Delta t, \quad (2.49)$$

$$x_{k+1} = x_k + \mathbf{v}_{k+1/2} \Delta t \quad (2.50)$$

This algorithm determines the new grain position with an error of order $O(\Delta t^4)$. But eq. 2.49 hides a difficulty in the application of this algorithm to granular materials (Radjai and Dubois, 2011). The problem is that the acceleration must be calculated at time $t = k\Delta t$. But the velocities are known at $t = (k - 1/2)\Delta t$, and not at $t = k\Delta t$. One way to get around this problem is to write

$$\mathbf{v}_k = \mathbf{v}_{k-1/2} + \mathbf{a}_{k-1} \Delta t / 2. \quad (2.51)$$

The equation uses the acceleration of the preceding time step to estimate the velocity. This approximation does not diminish the order of the algorithm. eq. 2.51 estimates \mathbf{v}_k with an error of order $\mathbf{O}(\Delta t^2)$, which produces an error of the same order in the calculation of the force in eq. 2.49. But this causes only an error of order $\mathbf{O}(\Delta t^3)$ in the velocity and an error of order $\mathbf{O}(\Delta t^4)$ in the position. However, this problem does not exist in energy conservation systems, because the computed forces do not depend on the velocities of the grains. The heaviest computational task is the evaluation of forces and not the integration of equations. The Verlet integration scheme is summarized in eq. 2.52 and figure 2.12. To calculate the forces and acceleration, it requires the positions and velocities at time t :

$$\begin{aligned} \mathbf{v}(t + \Delta t/2) &= \mathbf{v}(t - \Delta t/2) + \mathbf{a}(t) \Delta t, \\ x(t + \Delta t) &= x(t) + \mathbf{v}(t + \Delta t/2) \Delta t, \\ \mathbf{v}(t) &= \mathbf{v}(t - \Delta t/2) + \mathbf{a}(t - \Delta t) \Delta t / 2. \end{aligned} \quad (2.52)$$

The analysis of the Discrete Element Method formulation reveals that the linear force law gives the model a harmonic character, showing that it is very closely related to simple models widely used in physics and mechanics. The shortest time scales often arise from the

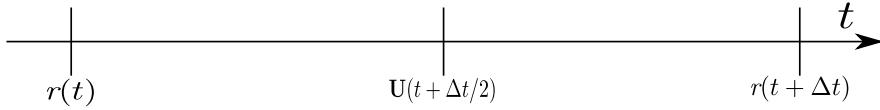


Figure 2.12 Verlet integration scheme

oscillations of one or two grains. The integration algorithm must resolve these movements with sufficient precision. Thus, the time steps used must be smaller than these time scales, the most rapid frequency is usually ω_N , the characteristic oscillation frequency of very short waves. This frequency is proportional to ω_0 , which is easier to estimate. Therefore, it is essential to choose a time step $\Delta t \approx \varepsilon/\omega_0$, where ε is a constant that depends on the integration algorithm. Values such as $\varepsilon \approx 0.01$ are often a reasonable choice (Radjai and Dubois, 2011). In the case of rapid granular flows, the time step must be small enough so that the fastest grains move only by a small fraction of their size during one time step. The grains must be stiff enough so that violent collisions do not lead to large overlaps between grains.

2.5.3 Boundary conditions

In many cases, the dynamic and static properties of a granular system are substantially affected by the interaction of the granular material with the system boundaries, i.e. by the properties of the container or the surface on which the material is present. The effect of boundary conditions on the response of the granular assembly can be noticed in the convective motion of granular material in vibrating containers, the formation of density waves in pipes, the motion of granular material on conveyors, and the clogging of hoppers. In these and many other cases, careful definition of the interaction between the granular material and the contact surface is essential. Of particular importance is the realistic modelling of the wall surface roughness. Unfortunately the mechanical interaction of granular materials with a rough wall is poorly understood (Poschel and Schwager, 2005). A simple way to define the wall property is to build up the wall from grains, which obey the same rules of interaction as the grains of granular material. By varying the size and position of the wall grains, system boundaries of adjustable roughness can be described. However, the surface roughness that characterizes the frictional properties of the wall has to be derived iteratively, and may not represent the real conditions. In the present case, a solid wall with corresponding stiffness, damping and frictional characteristics is introduced to model the interaction between grains and the wall. The interaction force is computed in a similar fashion to that of a pair of grains in contact and is divided into the normal and tangential components. The compression of the grain upon collision with the wall is calculated along the normal direction to the wall and the grain contact.

Periodic boundary

The effect of a wall on the response of grains is very critical, especially in numerical simulation where the number of grains is relatively fewer in comparison to the experiments. The undesired effect of a wall can be eliminated using periodic boundary conditions, i.e. a periodic extension of the simulation area in one or more dimensions. Any grain leaving the system at one side is reintroduced at the opposite side, and correspondingly the interaction forces between grains at opposite sides of the simulation area are taken into account. In this framework, the simulation domain becomes a unit area containing grains with periodic copies paving the whole system. The periodic boundary conditions extend the system boundaries to infinity, so that the simulation cell simply plays the role of a coordinate system to locate grain positions (see figure 2.13).

The external stresses or displacements are applied on the simulation box by constraining the degrees of freedom of the wall, which are alternatively kept free or fixed depending on whether a stress or a displacement is monitored in a system. With periodic boundary conditions, this role is played by the collective degrees of freedom carried by the coordinate system, whose basis vectors become dynamic variables, and their conjugate stresses are expressed as a state function of the granular configuration (Parrinello and Rahman, 1980). In the case of granular systems, there is dissipation of energy during grain interactions. The kinematics, equation of dynamics, and the time-stepping schemes for DEM are discussed in detail in Radjai et al. (2011). The periodicity in position implemented in the present study is discussed below.

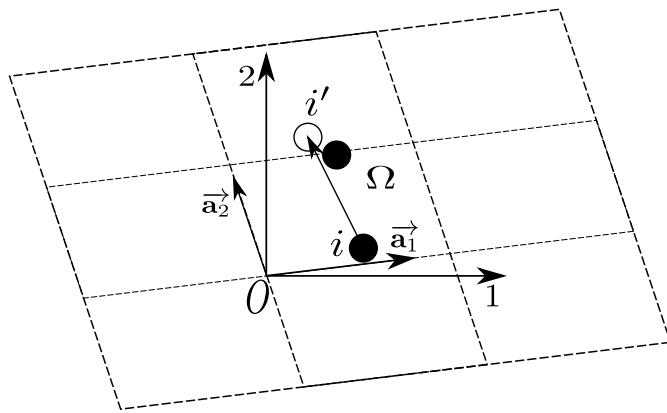


Figure 2.13 A 2D simulation cell ω with its basis vectors in an absolute frame. A grain located at the right boundary interacts with the image of another grain located at the left boundary.

Let us consider a collection of N_p grains with their centres contained in a cell of volume V . The cell can have any shape allowing for a periodic tessellation of space. The simplest shape is a parallelepiped i.e. parallelogram in 2D. The cell and its replicas define a regular

lattice characterized by its basis vectors (\vec{a}_1, \vec{a}_2). In the case of a parallelogram, the basis vectors may simply be the two sides of the parallelogram; figure 2.13. The origin O of the simulation cell is a vertex of the cell of coordinates $(0, 0)$ and its replicas are defined by two indices (i_1, i_2) corresponding to a translation of the origin by the vector $i_1 \vec{a}_1 + i_2 \vec{a}_2$. Then, the coordinates $\vec{r}(i')$ of the image i' of a grain $i \in \Omega$ of coordinates $\vec{r}(i)$ are given by:

$$\vec{r}(i') = \vec{r}(i) + \sum_{k=1}^2 i_k \vec{d}_k. \quad (2.53)$$

The grains belonging to the cell Ω , characterized by $i_1 = i_2 = 0$, can interact with the grains of the same cell but also with image grains in the neighbouring cells characterized by $i_k \in 1, -1$. There are $3^D - 1$ cells surrounding the simulation cell and they are involved in the search of contact partners for each grain. The distance between two grains i and $j \in \Omega$ is the shortest distance separating i from j or from one of its images j' . As the system evolves in time, a grain i may leave but one of its images i' enters at the same moment. In order to keep all original grains in the cell, the status “original” should be reserved to the grains whose centres belongs to Ω . Hence, whenever a grain i leaves the simulation cell, it becomes an image of i' , which then becomes the original. This means that a grain crossing a border of the simulation cell, returns to the cell by crossing another border.

2.5.4 Validation of DEM

It is essential to validate the developed DEM code. In the present study, a preliminary validation of the DEM code is performed by studying a ball rolling down an inclined plane. O’Sullivan et al. (2003) showed that the validation of DEM code using the above problem confirms the appropriate implementation of shear contact model in DEM. The theoretical solution for a ball rolling down an inclined plane is derived by Ke and Bray (1995). A disk is resting on a rigid inclined plane oriented at an angle $\beta = 45^\circ$ to the horizontal plane (figure 2.14a). The disk has a radius r of 1m and a density of 2650 kg/m^3 . The friction angle ϕ between the disk and the rigid plane is varied. The disk rolls/slides down the plane due to gravity. The DEM solution for the sliding case ($\phi = 0^\circ$) is compared with the theoretical solution by Ke and Bray (1995). The normal force, shear force, angular rotation, accelerations \ddot{a} and angular acceleration $\ddot{\theta}$ are compared with the theoretical solution (table 2.1). The accumulation of disk rotation at time $t = 0.2$ s versus the friction angle is presented in figure 2.14b. The angular rotation observed in the DEM matches the theoretical solution, which validates the shear contact model used in DEM. The DEM model implemented in

the present study is further validated by comparing it with the granular column collapse simulations performed by Zenit (2005) and using PFC2D (Itasca PFC2D, 1998).

Table 2.1 Comparison of theoretical and DEM result for a disk on an inclined plane of 45°

$\phi = 0^\circ$ (sliding)				
	$N = N/(mg \cos \beta)$	$S = S/(mg)$	\ddot{a}/g	$\ddot{\theta}/g$
Theoretical (Ke and Bray, 1995)	1.000	0.000	0.7071	0.000
DEM	1.000	0.000	0.7071	0.000

2.5.5 Cumulative β distribution

For a DEM analysis, the sample must be representative of the grain properties including the particle size distribution (PSD) both in volume (mainly for the smallest particles) and in number (for the largest particles). This representativeness of PSD is a condition for a sample to be a representative volume element. However, this condition cannot be satisfied in DEM for a poly-disperse sample, due to the upper limit on the computation capacity. It is important to extract a discrete ensemble of grain sizes such that a statistical representation of the size classes is obtained (Radjai and Dubois, 2011).

The β distribution in its cumulative form is able to satisfactorily model the size span (ratio of the largest to the smallest grain) and the shape descriptor (relative weights of the maximum and the minimum grain sizes). The cumulative β distribution (Voivret et al., 2007) is defined as

$$\beta(x, a, b) = \frac{1}{B(a, b)} \int_0^x t^{a-1} (1-t)^{b-1} dt, \quad (2.54)$$

where $a > 0$ and $b > 0$ are the two parameters of the distribution. The $B(a, b)$ function is given by

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}, \quad (2.55)$$

where Γ is the gamma function defined by

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt. \quad (2.56)$$

The cumulative β (CB) distribution is defined and normalised in the interval $[0,1]$ with $\beta(0) = 0$ and $\beta(1) = 1$. To represent the grading curve of grain size range $[d_{min}, d_{max}]$ with

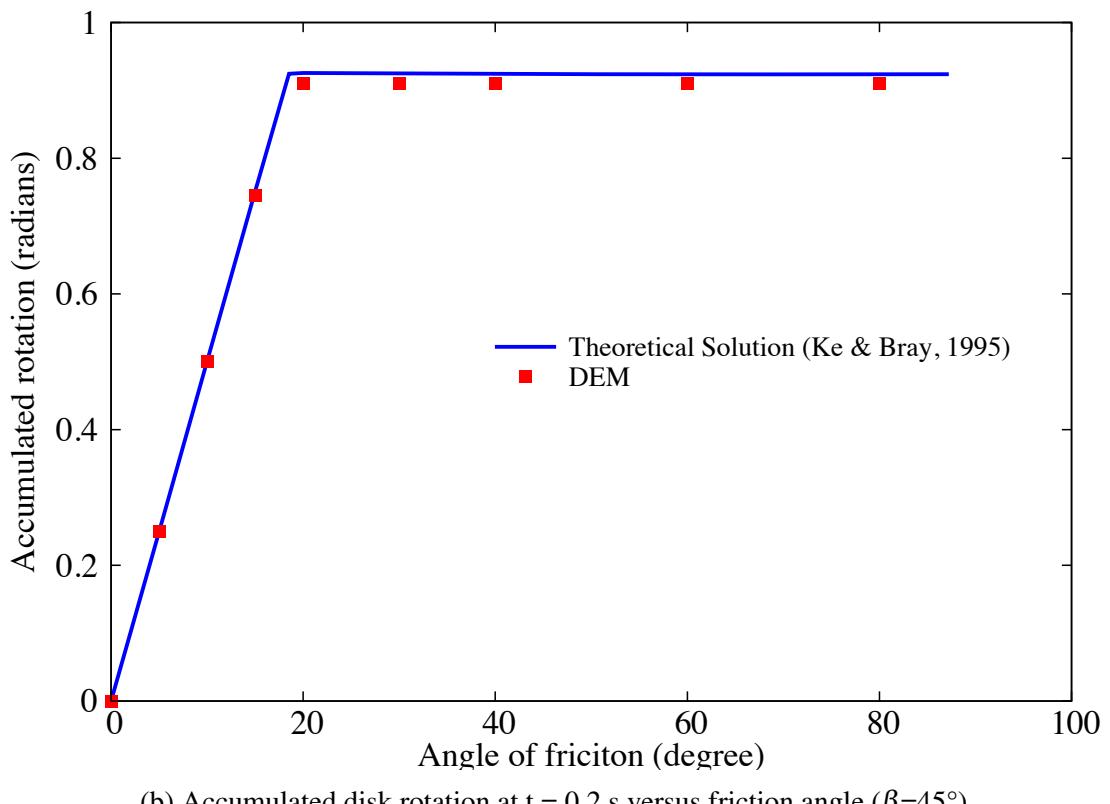
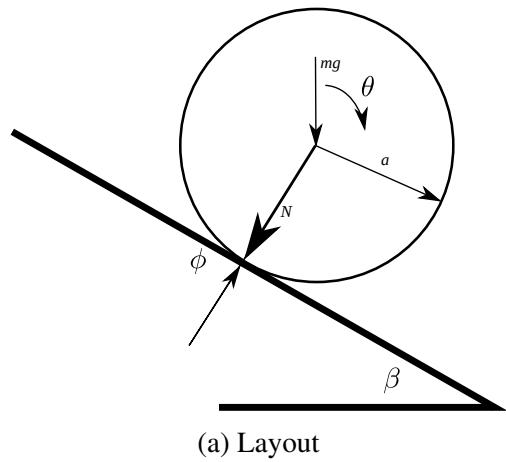


Figure 2.14 Validation of DEM using a disk rolling down an inclined plane

CB, the argument x is replaced by the reduced diameter d_r

$$d_r(d) = \frac{d - d_{min}}{d_{max} - d_{min}}, \quad (2.57)$$

which varies in the range of [0,1]. The model grading curve $h(d)$ is given by the CD distribution in terms of the reduced diameters as

$$h(d, a, b) = \beta(d_r(d); a, b). \quad (2.58)$$

The parameters a and b of the CB model allows the shape descriptor $h(d)$ to vary easily. The size span is characterised by the ratio $r = d_{max}/d_{min}$. The size span can also be defined as

$$s = \frac{d_{max} - d_{min}}{d_{max} + d_{min}}. \quad (2.59)$$

A value of $s = 0$ indicates a strictly mono-disperse grain size and a value of $s = 1$ indicates an infinitely poly-disperse grain size distribution. Voivret et al. (2007) observed a well graded particle size distribution for $a > 1$ and $b > 1$.

In the present study, a value of $a = 4$ and $b = 4$ is adopted to get a well graded curve. In the present study, samples with different poly-dispersity $r = 1.5, 1.8, 2$ and 6 are used. ?? shows a poly-disperse sample $r = 1.5$ generated using the CB method, for $a = 4$ and $b = 4$. The PSD curve of the generated sample is also presented.

2.5.6 Particle assembling methods

In order to simulate a granular assembly, it is essential to assign an initial position and velocity to all the grains in the system. Particle positions should be chosen to be compatible to the structure (granular fabric) we are trying to simulate. In any event, the grains should not be positioned such that there is an appreciable overlap between grains. In order to achieve the initial position of the grains, various grain-assembling methods can be adopted. The grain assembling methods can be classified into two broad categories: dynamic methods and geometrical approaches. The dynamic approach involves packing of grains using laws of mechanics and contacts, while in the geometrical method the grains are packed considering their geometry, i.e. grain size, shape and its position. In general, the packing of grains can be categorized into two types: crystal/lattice packing, like hexagonal or square pattern of mono-disperse grains, and random packing with varying density employing mono-disperse or poly-disperse grains. The crystalline packing arrangements, such as hexagon and square lattices, are easier to generate, however they have non-trivial effects on the response of the

granular system (Staron et al., 2005). Hexagonal packing is the densest possible arrangement for mono-dispersed spherical grains. In 2D, the packing of mono-dispersed circles on a hexagonal lattice yields a packing density, defined as the ratio of volume of solids to the total volume (V_s/V), of $\eta_h = \frac{1}{6}\pi\sqrt{3} \approx 0.9068$

The rheology of a granular material is controlled by the geometry of the assembly, which includes the grain shape, size distribution, and their arrangement. This prevailing role of geometry sometimes permits to simplify the dynamics in favour of a better description of the geometry and/or higher numerical efficiency (Radjai and Dubois, 2011). For example, a dense granular packing may be efficiently constructed by replacing the equations of dynamics by simple displacement rules satisfying the geometrical constraints. Purely geometrical procedures can be much simpler and numerically faster than dynamic or quasi-static methods. Contrary to dynamic simulation methods, the geometrical methods allow for quick assembling of a large number of grains. Such a packing may then be used as the initial state for dynamic simulations. The issue of the assembling methods is to construct configurations of grains as close as possible to a state of mechanical equilibrium with built-in packing properties. This can be a target packing density for a given grain size distribution. In the same way, the average connectivity of the grains (coordination number) and the anisotropy of the contact network are basic geometrical properties. The coordination number represents the mechanical response of packing. The homogeneity of the grain assembly in terms of packing fraction and connectivity is another important property, which depends on the assembling rules. In the present study, the initial grain packing is obtained using the ballistic deposition technique.

Ballistic deposition

Initially a random arrangement of grains which do not touch each other is generated. The radii of the grains are chosen from the interval of (R_{min}, R_{max}) in such a way that the total mass of all grains from a certain size interval is the same for all sizes, thus ensuring that neither larger nor smaller grains dominate the system. The grains are arranged randomly on a regular lattice. In the second step, the grains arranged in a regular lattice are allowed to fall down maintaining a constant potential head between layers of grains (figure 2.15).

The construction of the packing proceeds layer by layer from the substrate, hence this deposition model is also known as bottom-to-top restructuring model. In 2D, two contacts are sufficient to balance a grain if its centre of gravity lies between the two contacts. This corresponds to a position of local stable equilibrium. In this method, the order of deposited grains is generally random and independent of their sizes. The mechanically stable sample obtained from this method is presented in figure 2.16. Dense granular samples are prepared

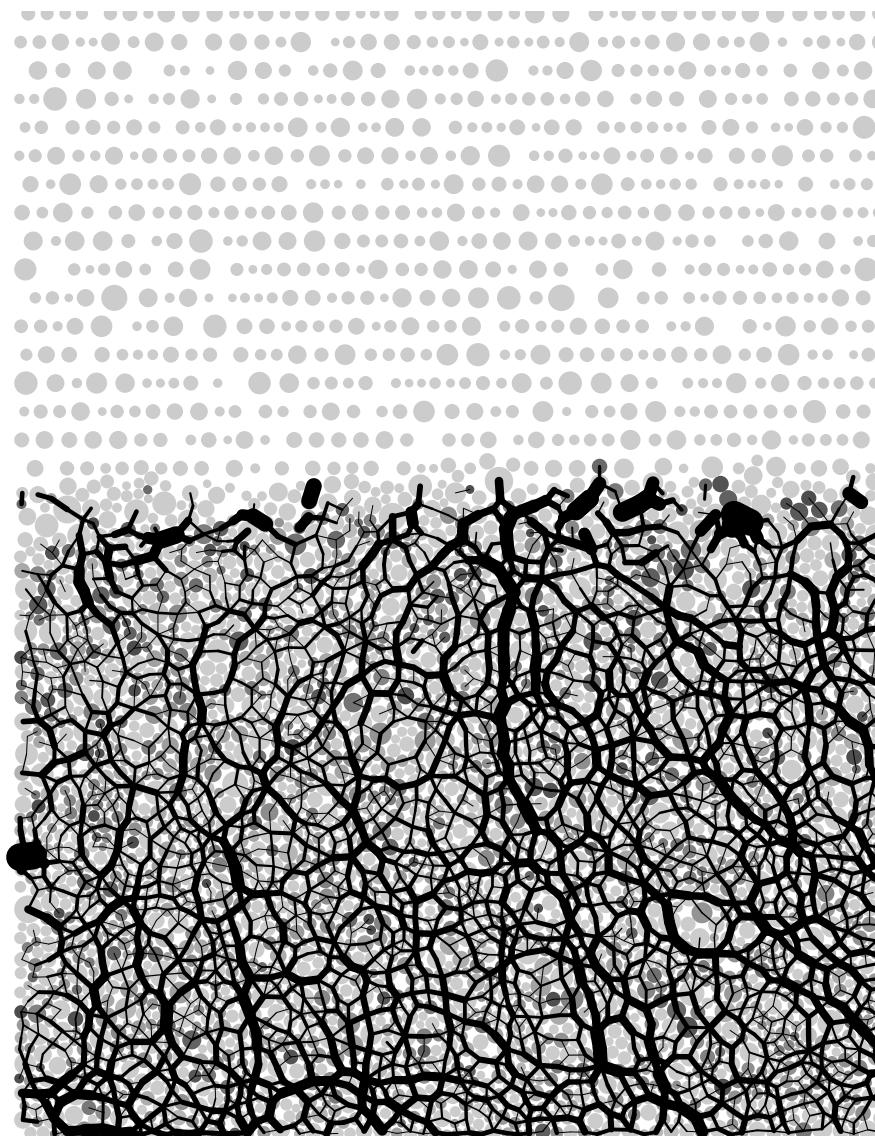


Figure 2.15 Generation of a poly-disperse sample using ballistic deposition technique

with zero initial friction angle. Zero frictional resistance ensures the densest possible packing. The friction angle is turned on during the analysis. To generate a dense sample, the sample is subjected to vibrations at varying frequencies.

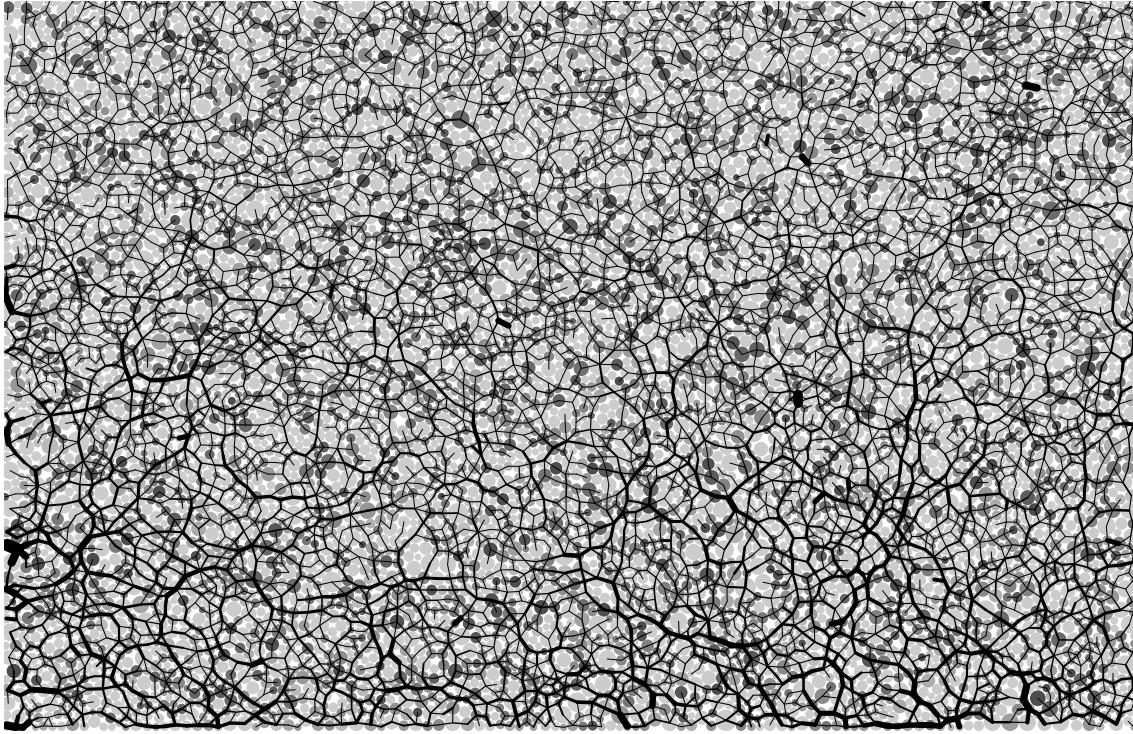


Figure 2.16 A poly-disperse DEM sample generated using ballistic deposition technique

Although there is no optimum specimen generation technique (O’Sullivan, 2011), there is a need to assess the homogeneity of the packing density generated (Jiang et al., 2003). The homogeneity of the sample is assessed by measuring the void-ratio within sub-volumes. The generated specimen is discretised into horizontal bands of $2.5d_{50}$. The homogeneity of the packing is calculated by the variance S in the void ratio.

$$S = \frac{1}{N_{layer} - 1} \sum_{i=1}^{N_{layer}} (e - e_i)^2, \quad (2.60)$$

where N_{layer} is the number of layers and e is the overall void ratio. A variance S of 2.74% is observed, which is less than 5% Jiang et al. (2003), indicating a homogeneous sample.

2.5.7 Voronoi tessellation

In order to extract bulk properties, such as packing density, stresses and strains, from a DEM simulation, it is important to quantify the granular texture. A useful geometrical

representation of granular texture consists of dividing the space occupied by the particles into contiguous cells. This procedure is called ‘tessellation’. Voronoi tessellation is one of the mostly commonly used technique. For a finite set of points p_1, \dots, p_n in the Euclidean space, the domain/plane is discretised into convex polygons such that each polygon contains exactly one point p_i and every point in a given polygon is closer to its generating point p_i than to any other. The inverse of the Voronoi tessellation is the Delaunay triangulation.

In the present study, the Fortune (1992) sweep line algorithm is implemented to tessellate the region surrounding each grain in the geometry. Once each grain has a corresponding area, the macroscopic properties such as the bulk density and stresses can be extracted from micro-mechanical properties such as the local packing density and force chains.

The Fortune sweep line algorithm involves a sweep line and a beach line, both of which move through the plane from left to right as the algorithm progresses. The sweep line is a straight line which moves from left to right across the plane. At any time during the algorithm, the points (grains) to the left of the sweep line will be incorporated into a Voronoi cell. While the points on the right of the sweep line are yet to be considered. The beach line is a complex curve, composed of pieces of parabolas that divides the plane within which the Voronoi diagram is known. As the sweep line crosses a point, a parabola evolves from the generating point. As the sweep line progresses, the vertices of the beach line, at which two parabolas cross, trace out the edges of the Voronoi diagram. The beach line progresses by keeping each parabola base exactly half way between the points initially swept over with the sweep line, and the new position of the sweep line. Figure 2.17 shows the Fortune sweep line algorithm in progress. In the present study, a modified version of the sweep-line algorithm is used to construct an additively weighted Voronoi diagram, in which the distance to each site (grain) is offset by the weight of the site, i.e., the radius of the grain.

The Voronoi tessellation is used to study the evolution of packing fraction during the collapse of a granular column. Figure 2.18a shows the Voronoi tessellation of the run-out for a granular column with an initial aspect ratio of 6 at time $t = 3\tau_c$. The distribution of local packing density for the run-out is shown in figure 2.18b. Dark regions represent dense packing, while loose regions are shown in white. The run-out at this stage has a bulk packing density of 81.23%. It is difficult to tessellate the free surface and the Voronoi cells on the free surface do not represent the actual packing density. Hence, during the evaluation of the macroscopic density, the packing density of surface grains that are larger than a threshold value are ignored. Voronoi Tessellation is a useful tool to extract continuum properties from DEM simulations. In the present study, the Voronoi tessellation is used to understand the evolution of packing density and entrainment of water in the flow front (due to hydroplaning) in granular flows.

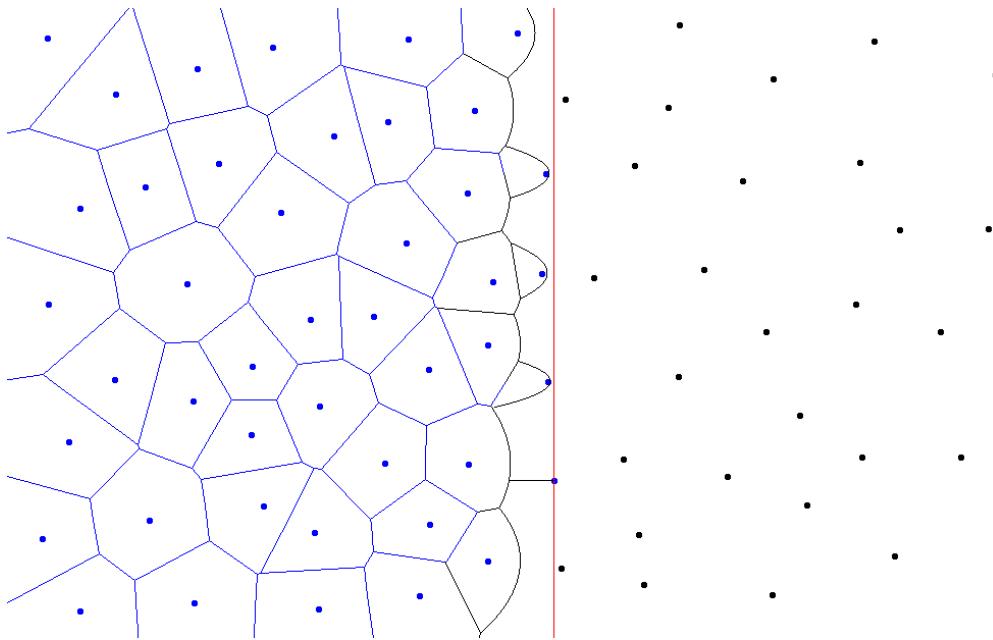


Figure 2.17 Fortune sweep line algorithm for generating Voronoi Tessellation. Generated from <http://www.diku.dk/hjemmesider/studerende/duff/Fortune/>.

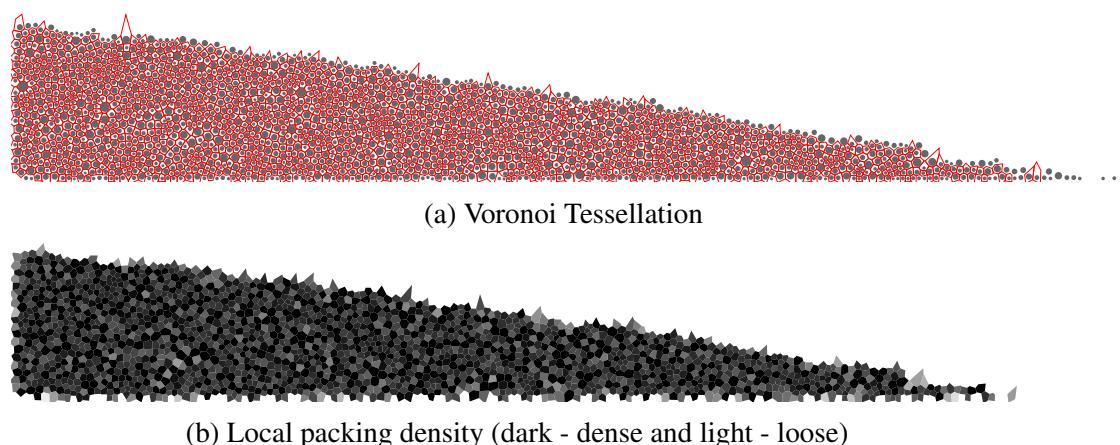


Figure 2.18 Voronoi tessellation of a run-out profile showing the local packing density

2.6 Summary

A plane-strain Material Point Method is implemented in the present study to describe the continuum response of granular flows. When the material points move from one cell to another, it results in numerical oscillations called as the cell-crossing noise. The Generalised Interpolation Material Point GIMP method is adopted to minimize these oscillations in large-deformation problems. The grain-scale response is captured using a two-dimensional DEM code. The discrete grains are generated using a cumulative β distribution, which mimics the particle size distribution curves. The sample is generated using the ballistic deposition technique and the homogeneity of the generated sample is verified by investigating the variance in the void-ratio at different layers. A sweep-line Voronoi tessellation approach is adopted to extract macroscopic parameters such as stresses and packing density from micro-scale properties such as the local packing fraction. These multi-scale tools are used to understand the rheophysics of dry granular flows and to evaluate the suitability of MPM as a continuum approach in modelling granular flow behaviour.

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