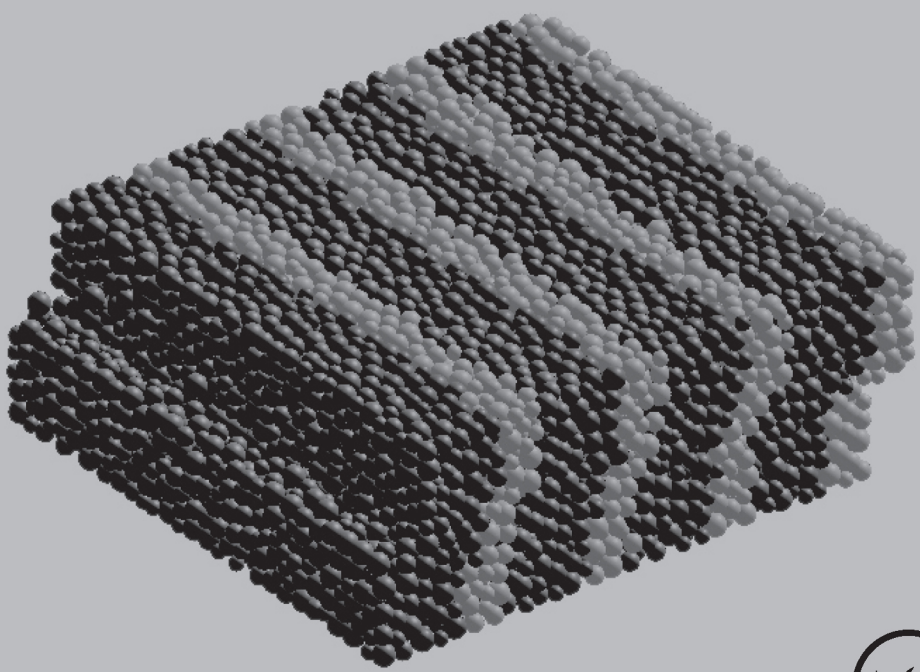
PARTICULATE DISCRETE ELEMENT MODELLING

A Geomechanics Perspective

CATHERINE O'SULLIVAN



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Particulate Discrete Element Modelling

This is the first dedicated work on the use of particulate DEM in geomechanics and provides key information needed for engineers and scientists who want to start using this powerful numerical modelling approach. The book is a concise point of reference for users of DEM, allowing them to maximize the insight they can gain their material response using DEM covering:

- The background theory
- Details of the numerical method
- Advice on running simulations
- Approaches for interpreting results of simulations
- Issues related to available particle types, contact modelling and boundary conditions.

Particulate Discrete Element Modelling is suitable both for first time DEM analysts as well as more experienced users. It will be of use to professionals, researchers and higher level students, as it presents a theoretical overview of DEM as well as practical guidance on how to set up and run DEM simulations and how to interpret DEM simulation results.

Catherine O'Sullivan is a Senior Lecturer in the Department of Civil and Environmental Engineering at Imperial College, UK. She obtained her undergraduate and master's degrees at University College Cork, Ireland. Dr. O'Sullivan's interest in DEM was sparked during her doctoral studies in Civil Engineering at the University of California at Berkeley, USA. Following graduation from UC Berkeley in 2002, she spent two years working as a lecturer at University College Dublin, prior to moving to Imperial College in 2004.

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a Geomechanics Perspective

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Acknowledgements

My objective in preparing this text is to introduce potential users to DEM, and to point them in the correct direction by collating in a single volume what I believe to be the important basic background information needed to develop the understanding needed to successfully complete DEM analyses and interpret the results from the analyses. While I have been carrying out research in this area for about the past decade, I am very aware that there are many other researchers who have more experience than me. However, following my own experience, I know it can be difficult and time consuming to identify the key elements of information necessary to have a handle on this field. I hope that this book will fill the current gap caused by the absence of a introductory text and so smooth the way for future DEM analysts.

My own knowledge of DEM has evolved over the past decade and many of my ideas have developed through interactions with colleagues and other researchers. My initial research at UC Berkeley was completed under the supervision of Prof. Jonathan Bray and Prof. Michael Riemer, and I also gained much from my interactions with other faculty and students at Berkeley, most notably Dr. David Doolin and Prof. Nick Sitar. All of my colleagues at Imperial College have been very supportive over the past six years. In particular my discussions with Prof. Matthew Coop have advanced my understanding of soil mechanics and helped form many of the ideas presented in this text and conversations with Dr. Berend van Wachem have advanced my understanding of DEM. Outside of my own institutions I would like to acknowledge Prof. Malcolm Bolton, Dr. Colin Thornton, Dr. Dave Potyondy and Prof. Stefan Luding who have been willing to engage in dis-

cussions on DEM and granular materials and who have been particularly generous in sharing their knowledge, opinions and ideas. I am lucky to have had the opportunity to work with a number of talented Ph.D. and Master's students over the past 8 years and I have learned a lot through discussions with these students. I would particularly like to thank my family who have been very encouraging of my academic career and who helped in the proof reading of this text, I could not have done this without their support.

Contents

Chapter 1

Introduction

1.1 Overview

Particulate DEM in geomechanics

Discrete element modelling (DEM) is a numerical modelling or computer simulation approach that can simulate soil and other granular materials. The unique feature of this approach is that it explicitly considers the individual particles in a granular material and their interactions. DEM presents an alternative to the typical approach adopted when simulating the mechanical behaviour of granular materials (soils in particular), which uses a continuum mechanics framework. In a continuum model soil is assumed to behave as a continuous material and the relative movements and rotations of the particles inside the material are not considered. Sophisticated constitutive models (i.e. equations relating the stress and strain in the soil) are then needed to capture the complexity of the material behaviour that arises owing to the particulate nature of the material. In DEM, even if simple numerical models are used to simulate the inter-particle contacts, and ideal, approximate, particle geometries are used, many of the mechanical response features associated with soil can be captured. Simplifying the particle shapes (e.g. using spheres) and adopting very basic models of the contact response reduces the computational cost of the simulation and thus allows systems involving relatively

large numbers of particles to be analysed while still capturing the salient response characteristics of soil behaviour.

There are a range of established and emerging numerical methods that can be used to simulate granular material response and so it is worth clarifying what the term "discrete element method" means in the context of this text. In a discrete element simulation a numerical model made up of a large number of discrete particles or bodies is created. A discrete element method is a simulation method where the finite displacements and rotations of discrete bodies are simulated (e.g. Cundall and Hart (1993)). Within the system it is possible for the particles to come into contact with each other and lose contact, and these changes in contact status are automatically determined. This definition excludes from consideration the meshless or meshfree continuum methods including smoothed particle hydrodynamics (SPH). In these methods the "particles" are interpolation points, rather than being physical particles, and so they are very similar to the nodes in a finite element model.

Particulate DEM is used across a variety of disciplines, ranging from food technology to mining engineering, however the seminal publication in this area by Cundall and Strack (1979a), was published in a soil mechanics journal (*Géotechnique*). Interest in the method amongst geotechnical engineers has grown since this original publication, with a marked increase in interest in recent years as a result of the increase in computing power.

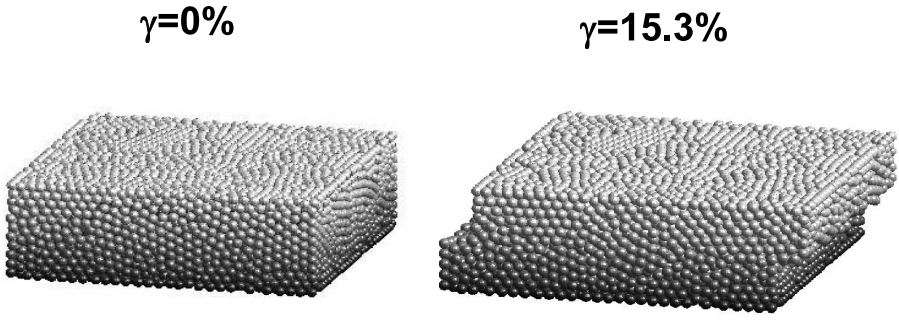


Figure 1.1: Simulation of a direct shear test using DEM

There are two main motivations to use DEM amongst both researchers and practitioners in the area of geomechanics. In the first case, in a DEM model, loads and deformations can be applied to virtual samples to simulate physical laboratory tests, and the particle scale mechanisms that underlie the complex overall material response can be monitored and analysed. In a DEM model the evolution of the contact forces, the particle and contact orientations, the particle rotations, etc., can all easily be measured. It is incredibly difficult (and arguably impossible) to access all this information in a physical laboratory test. Figure 1.1 illustrates a simulation of a direct shear test using particulate DEM. The DEM model allows us to look inside the material and understand the fundamental particle interactions underlying the complex, macro-scale response. To date knowledge of soil response has relied largely on empirical observation of the overall material response in laboratory and field tests. DEM simulations thus present geotechnical engineers with a valuable set of tools to complement existing techniques as they seek to develop a scientifically rigorous understanding of soil behaviour with likely improvements in our ability to predict response in the field. DEM therefore is now established as an essential tool in basic research in geomechanics.

A second, more applied, motivation for the use of DEM is that it allows analysis of the mechanisms involved in large-displacement problems in geomechanics. These problems cannot easily be modelled using more widespread continuum approaches such as the finite element method. Figure 1.2 illustrates a two-dimensional DEM simulation of the insertion of a cone penetrometer into a container of 117,828 disks (for details refer to Kinlock and O'Sullivan (2007)). The particles are shaded according to the amount of rotation they experience, with the particles distant from the penetrometer coloured white as they experience little disturbance, and those closest to the cone penetrometer (coloured black) being rotated and displaced during the penetration. This figure indicates that DEM can effectively accommodate the large displacements involved in the penetration mechanism. Failures in geomechanics often involve very large displacements or deformations, DEM models can therefore inform our understanding of important fail-

ure mechanisms. Examples of mechanisms that cannot be simulated using a continuum approach include internal erosion, scour and sand production in oil reservoirs. Figure 1.3 shows a bridge that collapsed in Ireland in 2009 following scour of its foundations, highlighting the importance of being able to simulate this class of problem.

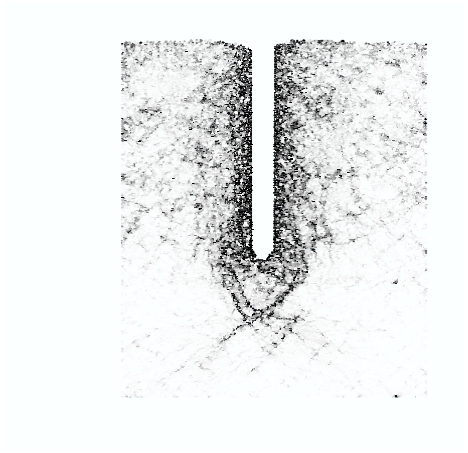


Figure 1.2: Two-dimensional DEM simulation of cone penetrometer penetrating a granular material (disk shading indicates magnitude of rotation)

Outline of book

The objective of this book is to serve as an introduction to the use of discrete element modelling to analyse the response of granular materials, focussing on applications in soil mechanics and geotechnical engineering. The intended audience is people who are thinking about using DEM, or people who are just starting to use DEM, rather than those with years of experience. However, hopefully users with some experience and DEM code developers will also find aspects of the text interesting and useful. In any case, it is assumed that someone interested in DEM is likely to be a graduate or post graduate engineer or scientist with some idea

Figure 1.3: Collapse of railway bridge in Malahide, Dublin, Ireland in August 2009, *Photo Courtesy Sarah McAllister*

of the basic principles of numerical modelling and a knowledge of mechanics.

The overall aim is to provide answers to a few key questions:

1. What is the theoretical basis of DEM ? What is the fundamental modelling approach used? (Chapters 2, 3, 4 and 6).

2. How does someone run a DEM simulation and what information can they get from it? (Chapters 5, 7, 8 and 11).

3. How do you interpret data from a DEM simulation? (Chapters 9 and 10).

4. What has already been achieved using DEM? (Chapter 12).

There is an emphasis on soil mechanics-related applications; however much of the content of this book has a broader application and should prove useful to those working in the fields of in powder technology, chemical engineering, geology, mining engineering, physics, and other disciplines where there is interest in analysing material response at a particulate scale. There are many particulate discrete element codes in use at present, some of which have been developed by individuals solely for research applications, while others are commercially available. This book is

not written with any particular code in mind, rather the material and discussions presented here should be of interest to users (and possibly developers) of many different codes.

This initial Chapter aims to introduce the general principles of DEM and presents some of the mathematical concepts used in later Chapters.

1.2 Particulate Scale Modelling of Granular Materials

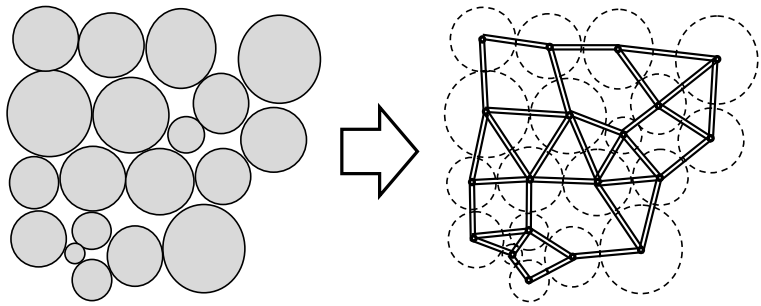


Figure 1.4: Analogy between a granular material and a highly complex, statically redundant structural frame

In discussing the need for computer simulation to facilitate analysis of particulate systems at the micro-scale, Rapaport (2004) points out the similarity between the interaction of a large system of particles and the classical "n-body" problem that has attracted the attention of physicists for hundreds of years. The n-body problem considers the evolution of a system of n "bodies" subject to Newtonian gravitational forces. The initial motivation to analyse this problem was a desire to understand the dynamics

of the solar system. There is no general closed-form solution to this problem for systems with more than 3 bodies, consequently numerical methods and computer models are required to analyse these systems.

The need to adopt a computer-based model to analyse granular materials at the particle scale can be appreciated by looking at the system from the perspective of a structural engineer. As illustrated in Figure 1.4, an analogy can be drawn between an assembly of contacting particles and a structure with many elements connecting the nodes of the structure. Engineers, in particular civil engineers, understand that a structure with a large number of connections is statically indeterminate. In a statically indeterminate structure, the forces in each structural member cannot be calculated by considering the static equilibrium of the system alone. More more sophisticated (and nowadays) computer-based models that include consideration of the deformations and hence the stiffness of the structural elements are required to determine the forces within the structure.

Both Duran (2000) and Zhu et al. (2007) divide the numerical techniques used in DEM into two categories called *soft sphere* models and *hard sphere* models. A major differentiation between the methods in each category is whether the particles are approximated to be "soft", in which case penetration is allowed at the particle contacts or "hard", when no deformation or penetration is considered. Figure 1.5 illustrates schematically both approaches. Both types of simulation are transient, or time dependent. This means that the evolution of the system over a period of time is considered by examining the state of the assembly of particles at distinct time intervals.

The hard particle, or hard sphere, approximation is at the basis of the so-called "collisional" or "event driven" (ED) models. The word *hard* refers to the absense of interpenetration or deformation during impact of particles. The collision itself is not necessarily of interest and may be assumed to be instantaneous. The ED models start from the equations governing momentum exchange and the particle contact force is often not explicitly considered (Zhu et al., 2007). This type of model recognizes that when particles collide

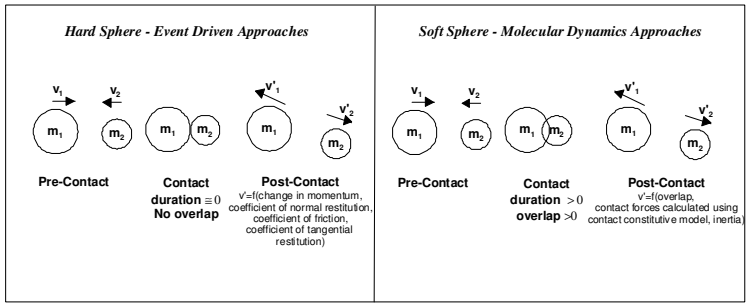


Figure 1.5: "Hard Sphere" and "Soft Sphere" approaches to DEM

energy is dissipated by plastic deformation and heat. The resultant loss of momentum when a collision occurs is characterized solely by means of the coefficients of elastic restitution. Different values for the normal and tangential coefficients of restitution are specified.

Event driven algorithms analyse events sequentially in the order in which they occur. This means that at any time during the simulation at most only one collision can occur at a given time in the analysis. The time increment used in the simulations varies, and equals the time between one collision and the next. Between collisions the particles move along a uniform trajectory.

Applications suited to the use of the event driven modelling approach are generally those involving rapid granular flow, where the granular material has been partially or completely fluidized, e.g. avalanches, or rapid flow through conduits in manufacturing processes. For example, Hoomans et al. (1996) used this approach to simulate fluidized beds for process engineering applications, and Campbell and Brennan (1985) used a hard sphere approach to simulate granular material flow. Delaney et al. (2007) correctly argue that, while it is computationally cheaper than other methods, the hard sphere approach fails to capture the fine details of the response of dense materials involving multiple simultaneous contacts. Delaney et al. also highlight the limitation in the ability to accurately model the tangential or frictional forces between interacting particles. Campbell (2006) considered this method to be inappropriate for considering dense systems as it is non-physical:

the real mechanism of force transfer in a granular material involves deformation of the contacting particles. For further information on event driven approaches refer to Brilliantov et al. (2996) or Rapaport (2009). Pöschel and Schwager (2005) describe two alternative algorithms for implementation of an event driven computer code. As hard sphere approaches are not commonly considered in current geotechnical engineering research or practice, they are not considered further here.

The principle behind the soft sphere approach is to solve, in increments of discrete time, the equations governing the linear and angular dynamic equilibrium of the colliding or contacting particles. This contrasts with the strategy used in ED models, which start from the equations governing momentum exchange. The word "soft" is a misnomer; the particles in the "soft sphere" simulations are rigid, however they can overlap at the contact points. (As discussed above, no overlap is allowed in the "event driven" methods.) In this approach, friction and elastic restitution come into effect only when spheres penetrate each other. In the soft sphere models, the normal component of the inter-particle force is calculated considering either the particle overlap at the contact point (for compressive forces) or the particle separation at the contact point (where tensile force transmission occurs). In geomechanics applications in particular, a key assumption is that the compressive overlap or tensile separation will be small. The shear or tangential forces are calculated from the cumulative relative displacement at the contact points in a direction orthogonal to the contact normal orientation. In contrast to the hard sphere approach where only one collision is considered at each time increment, the soft sphere models can handle systems with multiple simultaneous contacts, as typically arise in static or quasi-static problems. As outlined by O'Sullivan (2002), various algorithms that fall within this "soft sphere" category exist however, the most commonly used approach is the *distinct element method*, as originally described by Cundall and Strack (1979a). Given the prevalence of Cundall and Strack's approach the terms "discrete element method" and "distinct element method" are essentially used interchangeably. Strictly speaking the distinct element method really is

a type of discrete element method. The distinct element method is the method given the most consideration in this text. Other soft sphere approaches that are algorithmically similar to DEM include the discontinuous deformation analysis method (DDA) (Shi (1988), adapted for particle systems by Ke and Bray (1995)), and the implicit methods proposed by Kishino (1989) and Holtzman et al. (2008).

There are a few documented geomechanics research studies that have adopted a method called contact dynamics (e.g. Lanier and Jean (2000)). This method does not strictly fall within either the event driven or soft sphere frameworks and is sometimes referred to as rigid body dynamics (Pöschel and Schwager, 2005). The general idea is that the contact forces between the particles are determined so that there is no particle deformation (i.e. "hard spheres", but with finite contact durations). The tangential forces are determined by considering the forces required to keep the particles from sliding. Pöschel and Schwager (2005) state that while the algorithm associated with this method is more complex than DEM or molecular dynamics, and there are more calculations involved in each time increment, there is not a corresponding increase in computational cost, as the time increments in the analysis are larger.

Another particle-scale approach that is used to analyse granular materials is the Monte Carlo method. As in the event driven approach, penetration of particles is not allowed; however the contacts are finite in duration. As outlined by Sutmann (2002), amongst others, in this simulation approach at each iteration each particle is subject to a number of trial moves. The change in energy generated by each of these moves is calculated and the movement leading to the lowest energy is that selected for progressing to the next configuration. This approach is applicable only to the study of systems in static equilibrium, i.e. it cannot be applied to consider flow of granular materials. A less well-established statistically based approach involving the application of the Markov stochastic process was described by Kitamura(1981a,b).

Molecular dynamics

It is important to be aware of the similarities between particulate DEM and molecular dynamics. Molecular dynamics is an analysis tool used in chemistry, biochemistry and materials science. Using this method, materials are studied at the most fundamental level by simulating the interactions between individual molecules or atoms. The objective of these simulations is to relate the bulk properties of a material (be it liquid, solid or gas) and fundamental atomistic interactions. These particles are modelled as point-like centres that interact via pair or multi-particle interaction potentials (e.g. the Leonard-Jones potential). The time scales of interest in molecular dynamics are of the order of 1 μs, and the trajectory lengths are between 10 and 100 Ångstroms (Sutmann, 2002).

Liquids tend to be the materials most commonly considered in molecular dynamics simulations, with consideration often being given to analysis of phase transformation, for example. In fact the method was initially proposed by Alder and Wainwright (1957) who described the phase transformation of a system of rigid spheres, these authors later outlined the general methodology of molecular dynamics in Alder and Wainwright (1959). Sutmann (2002) outlines the history of molecular dynamics, while Rapaport (2004) provides an overview of molecular dynamics, including details of the implementation of a molecular dynamics code. Pöschel and Schwager (2005) suggest that typical molecular dynamics simulations are less computationally intensive than particulate DEM simulation as in DEM the particles exert forces on each other only when they are in contact. The numerical stability requirements necessitate a smaller time step for particulate DEM as the contact response is relatively stiff (the influence of contact stiffness on the simulation time increment is considered in some detail in Chapter 2). However, some molecular dynamics methods (ab initio molecular dynamics) consider explicitly the interaction of the particles at the electron scale and are significantly more complex than granular DEM (e.g. the ONETEP algorithm proposed by Skylaris et al. (2005)).

As noted above meshless methods, including SPH, are another

type of particle-based model used in geomechanics. The basic idea in meshless methods is that the "particles" are used as interpolation points where the material displacement is tracked, and the material is continuous between these points. These methods differ significantly from the particulate DEM methods considered in this text and they are not given further consideration here. Readers seeking additional information on the meshless methods may wish to refer to Belytschko et al. (1996).

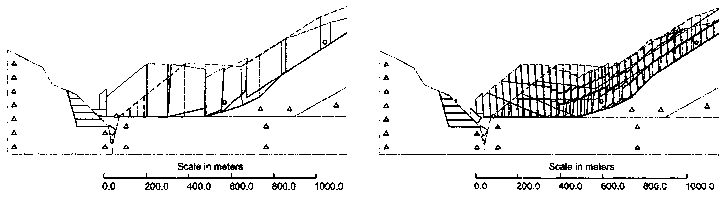
1.3 Use of Block DEM Codes in Geomechanics

Two types of discrete element model are used in geomechanics, referred to here as block DEM and particulate DEM. Both types of model considers systems made up of numerous individual bodies, either blocks or particles. These discrete bodies can move relative to each other and they can rotate. Contacts can form between the bodies, and as the system deforms, these contacts can break and new contacts can form. Typically a small amount of overlap is allowed at the contact between the bodies, and this overlap is analogous to the deformation that occurs at the contacts between the real bodies. Simple "contact constitutive models" are used to relate the contact forces between the bodies to the contact overlap. The shear components of the contact force impart a moment to the bodies. Knowing the contact forces and the inertia of the body, by considering the dynamic equilibrium of each body, its acceleration can be calculated. From these accelerations, displacements of the particles over small time increments can be determined. By advancing forward using these small time steps the evolution of the system can be simulated.

While the focus of this book is on particulate DEM, it is important to be aware of the use of block DEM simulations in geomechanics. This type of analysis is used to model systems of polygonal rock blocks or masonry structures; for example Powrie et al. (2002) analysed dry stone retaining walls, while Basarir et al. (2008) simulated excavation of rock. Examples of block discrete

element codes include the commercial code UDEC (Itasca (1998)) and the Discontinuous Deformation Analysis code (DDA) (e.g. Shi (1988), MacLaughlin (1997), Doolin (2002)). In these codes a system of orthogonal, stiff ("penalty") springs are used to calculate the contact forces, while minimizing the overlap between the blocks. The blocks are typically simply deformable (linear elastic). The ability of the blocks to deform is the principal difference between the block codes and the particle codes. As a consequence of the block deformability, for two equivalent simulations using the same number of particles and same particle geometries, the calculations are more time-consuming in comparison with a simulation using a particle code with rigid particles.

Figure 1.6 illustrates the application of the DDA block code to analyse the Vaiont landslide that took place in Italy in 1963. As described by Sitar et al. (2005), when compared with limit equilibrium analyses, the DDA simulations yielded reasonable results and facilitated parametric studies considering the influence of the number of discontinuities on the deformation mode. This approach to discrete element modelling is not considered in detail in this text, however many of the basic principles underlying the particulate discrete element modelling codes described here also apply to block discrete element codes.



(a) 12 block discretization

(b) 105 block discretization

Figure 1.6: Back analysis of Vaiont Landslide using the Block Discrete Element Method, DDA. *Solid lines indicate deformed block configuration, dashed lines indicate original slope geometry.* Sitar et al. (2005)

1.4 Overview of Particulate DEM

As noted above, the distinct element method is the type of discrete element method that is currently most popular in geomechanics. The basic formulation for the distinct element method for granular materials was proposed and described by Peter Cundall and Otto Strack in two reports to the US National Science Foundation, Cundall and Strack(1978 and 1979b) and a subsequent paper in the journal *Géotechnique* (Cundall and Strack, 1979a).

An overview of the sequence of calculations involved in a DEM simulation is given in Figure 1.7. To carry out a DEM simulation initially the user inputs the geometry of the system to be analysed, including the particle coordinates and boundary conditions. The material properties are usually input by specifying the contact model parameters, including stiffness and friction coefficient. The user specifies a schedule for loading or deforming the system. Then the simulation progresses as a transient, or dynamic, analysis, typically for a specified number of time increments. At each time step the contacting particles are identified. The magnitude of the inter-particle forces relate to the distance between contacting particles. Having calculated these inter-particle forces, the resultant force and moment or torque acting on each particle can be determined. Except when particle rotation is inhibited, at each time increment two sets of equations for the dynamic equilibrium of the particles are solved. The translational movement of each particle is determined from the resultant applied force, and the resultant applied moment is used to calculate the rotational motion. Knowing the particle inertia, the translational and rotational accelerations of the particles can be calculated. The displacement and rotation of the particles over the current time-step is then found through a simple central-difference-type integration through time. The resultant forces and moments that impart these translational and rotational accelerations on the particles are sometimes called "out-of-balance" forces (e.g. Thornton and Antony (2000), Itasca (2004)). Using these incremental displacements and rotations, the particle positions and orientations are updated, in the next time step the contact forces are then calculated using this

updated geometry, and the series of calculations are repeated. A discrete element analysis is therefore a transient or dynamic, analysis, even if the system of interest is responding in an almost static manner.

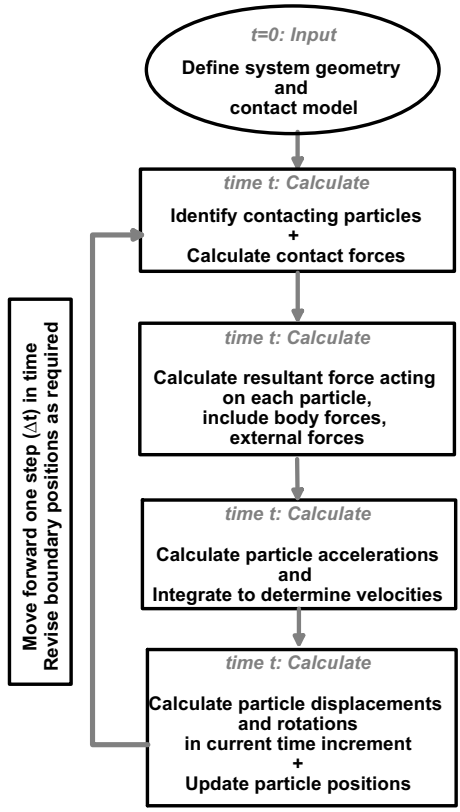


Figure 1.7: Schematic diagram of sequence of calculations in a DEM simulation

As illustrated in Figure 1.8 within each time increment there are two main series of calculations. In the first instance the particle velocities and incremental displacements are calculated by considering the equilibrium of each particle in sequence. Then having updated the system geometry the forces at each contact in the system are calculated. The tangential component of the contact force will always impart a rotational moment to the particles,

and in many cases the normal contact force component will also generate a moment. These forces and moments are distributed to the particles and then used to adjust the particle positions in the next time increment.

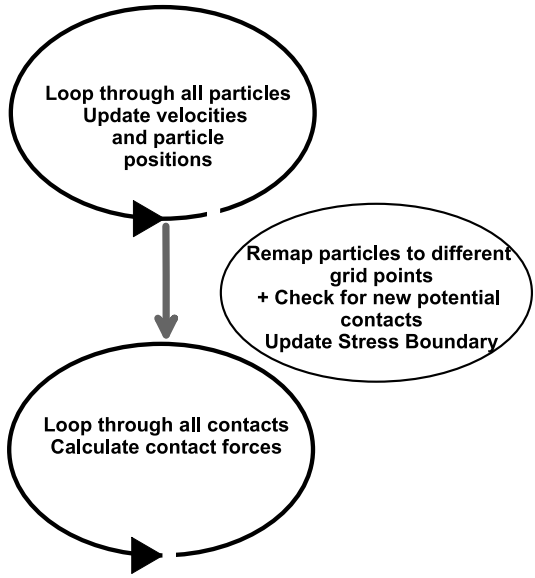


Figure 1.8: Indication of calculation sequence within a DEM time step

A clear statement of the assumptions inherent in DEM is important from the outset, although it must be acknowledged that not every implementation of DEM may adhere exactly to these assumptions, particularly as the complexity of DEM codes increases. However, using the lists proposed by Kishino (1999) and Potyondy and Cundall (2004) as a basis, the following key assumptions typically made in particle-based DEM simulations can be stated:

1. The basic particles are rigid, they possess a finite inertia (mass and rotational inertia) and they can be analytically described.

2. The particles can move independently of each other and can translate and rotate.

3. The program automatically identifies new contacts between particles.

4. The contact between particles occurs over an infinitesimal area and each contact involves only two particles.

5. The particles are allowed to overlap slightly at the contact points and this overlap is analagous to the deformation that occurs between real particles. The magnitude of the deformation of the each particle at the contact point is assumed to be small.

6. The compressive inter-particle forces can be calculated from the magnitude of the overlap.

7. At the contact points, it is possible for particles to transmit tensile and compressive forces in the contact normal direction as well as a tangential force orthogonal to the normal contact force.

8. Tensile inter-particle forces can be calculated by considering the separation distance between two particles. Once the tensile force exceeds the maximum tensile force for that contact (which may be 0), the particles can move away from each other and the contact is deleted and no longer considered when calculating the contact forces.

9. The time increment chosen in a DEM simulation should be small enough that the motion of a particle over a given time step is sufficiently small to only influence its immediate neighbouring particles.

10. Agglomerates of the rigid base particles can be used to represent a single physical particle, and the relative motion of these base particles within the agglomerate may cause a measurable deformation of the composite particles. Alternatively these agglomerates may themselves be rigid.

From the analyst's point of view there are many similarities between the overall process involved in a DEM simulation and the

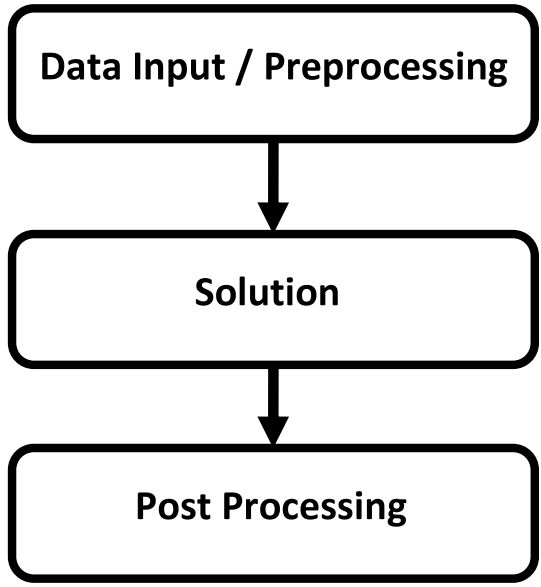


Figure 1.9: Generic Flow Chart for Numerical Analysis in Mechanics

process involved in a continuum-based analysis, e.g. using finite element analysis. A generic flowchart for numerical analysis in mechanics is given in Figure 1.9. There are some key differences between the effort associated with a DEM analysis and a conventional continuum analysis. Undoubtedly mesh generation for finite element analysis of bodies with highly complex geometries is non-trivial. However, t generating the initial positions of the particles in the problem domain to be analysed is probably more difficult and typically involves DEM calculation cycles. In fact, it is possible for this model creation phase to be at least as computationally expensive as the main simulation. As calculation cycles are involved in the specimen generation stage, the discussion of this phase of the analysis is given in Chapter 7, after the details

on the method have been considered in Chapters 2–5.

The non-linearity of the systems considered and the explicit approach to time integration used mean that a small time increment must be adopted in DEM simulations. It is these considerations, combined with the need to include large numbers of particles, that make DEM simulations so computationally intensive.

A DEM simulation generates basic results in terms of individual particle positions and inter particle contact forces, rather than in terms of stress and strain. A postprocessing procedure is required to interpret these results in a useful or meaningful manner and relate them to our continuum-mechanics based understanding of soil behaviour. A wide variety of interpretation techniques have been proposed in the literature, some of which are not easy to implement and typically involve greater effort and more abstract concepts (including statistical mechanics) than the methods used to interpret continuum analyses. Chapters 8–10 provide overviews of various interpretation approaches.

For readers accustomed to continuum-based geomechanics analyses it may be useful to consider how DEM meets the theoretical requirements for a valid analysis. In conventional continuum mechanics a method of analysis is typically required to satisfy four theoretical requirements, namely equilibrium, compatibility, constitutive behaviour and boundary conditions. In a DEM simulation equilibrium is accounted for by considering the dynamic equilibrium of each particle at each time increment during the analysis. As discussed further in Chapter 11, for quasi-static analyses the user must also consider the overall equilibrium of the system as a test to establish the validity of a particular simulation. In a continuum analysis the compatibility requirement is satisfied, meaning that as the system deforms holes should not appear and the material does not develop overlaps. As outlined by Potts (2003), amongst others, from a mathematical perspective this requirement implies that components of strain exist and are continuous and the derivatives of strain exist to at least second-order. This requirement is effectively violated in a particulate DEM simulation. No strain occurs within the rigid bodies, they are allowed to overlap and the displacement field is highly non-uniform. A discussion on

interpreting DEM analysis by calculating strains from the particle displacements is given in Chapter 9.

In continuum-based materials modelling, the constitutive matrix relates the stresses and strains within the material and this relationship can be linear or non-linear. No constitutive model is required in a DEM model; rather, as discussed in many DEM related papers, the constitutive model "emerges" from the DEM simulation results. A model describing the response at the particle contacts is required and this is somewhat analogous to the constitutive model. A direct mapping of the contact model to a continuum constitutive model would be inappropriate. The macro-scale or continuum response will depend on the response at the contacts, the geometry of the granular material and the ability of the particles to crush, fail or deform. Even if a linear contact model is adopted, the overall response will be non-linear as a consequence of the evolution of the inter-particle contacts.

Finally a statement of the boundary conditions is required; these boundary conditions play a large role in defining the problem to be analysed. The concepts of boundary conditions are similar in both continuum and DEM analyses; however, the details differ and a discussion on the various boundary conditions used in DEM simulations is given in Chapter 5.

1.5 Use of DEM Outside of Geomechanics

Granular materials are encountered in a variety of disciplines outside of soil mechanics and geotechnical engineering. Most notably, chemical and process engineers also regularly adopt DEM in their research. The complexity of granular material response has attracted interest from mathematicians and physicists who use DEM simulations to generate data for subsequent detailed analysis of the fundamentals of granular material response. As in the case of geomechanics applications, there is potential, with increasing computational power, to apply DEM to solve industrial problems. Recent conference proceedings, e.g. Nakagawa and Luding (2009),

illustrate the range of applications of DEM across these disciplines. Much information on the applicability of DEM to advance understanding of granular materials for geomechanics applications can therefore be gained by reference to journals in these other disciplines. Two particularly useful publications are Zhu et al. (2007 and 2008) which provide reviews of the development of DEM algorithms and the application of DEM respectively from a chemical engineering perspective. The recent special editions of the journals *Powder Technology*, Thornton (2009), and *Particuology*, Zhu and Yu (2008), also contain papers of interest to the geomechanics community.

1.6 Introduction to Tensorial Notation

Tensorial notation (sometimes called index notation) is adopted throughout this book. Most publications referred to in the book also use tensorial notation and, while some authors (e.g. Potyondy and Cundall (2004)) provide clarification, familiarity with this notation tends to be assumed. This section is included to give the reader a very brief overview of tensorial notation both to facilitate understanding of the material in this book as well as the broader set of publications associated with the topic. For more detailed explanation reference to a continuum mechanics textbook (e.g. Shames and Cozzarelli (1997)) is recommended.

Tensorial notation is attractive as it is allows vectors and operations on vectors to be described concisely. It has particular advantages when developing computer programs where data are stored in arrays that are accessed using integer indices. In particulate DEM there are calculations and operations involving force vectors, position vectors, displacement vectors, etc. In this book the intrinsic form of the vector is denoted in bold typeface; thus the particle displacements are given by $\mathbf{u}$, the resultant force acting on a particle is given by $\mathbf{f}$, and the particle position is given by $\mathbf{x}$. These terms are then used to refer to the vectors in a general sense as entities with a specific magnitude ($|\mathbf{u}|$ or $|\mathbf{f}|$) and whose directions can be described relative to a specified coordinate sys-

tem.

Every vector will have components parallel to each of the coordinate axes. Tensorial notation provides a convenient means of describing operations on each of these components. When these vectors are expressed in tensorial, or indicial, form they are denoted u_i, f_i and x_i with the subscript i indicating that the vector component parallel to a specific coordinate axis, i, is under consideration. For example, if the term u_i is used to describe the displacement of a particle, this vector may have either 2 or 3 components, depending on whether we are considering a two-dimensional or three-dimensional analysis. In the Cartesian coordinate system the displacement denoted u_i is given by $u_i = (u_x, u_y)$ and $u_i = (u_x, u_y, u_z)$ in two-dimensional and three-dimensional analyses respectively. As there is only one index (i) the vector u_i is a first-order tensor.

Extending consideration to two-dimensional tensors, the stress tensor is given by $\boldsymbol{\sigma}$ or σ_{ij} and this tensor can represent either a two-dimensional or three-dimensional state of stress. In this case, even if the stress state is fully three-dimensional, there are two indices (i and j) and this tensor is then a second-order tensor. The indices i and j are considered "free indices" as they are both "free" to adopt independently any of the values x, y (and z in 3D). The stress tensor for two-dimensional analysis is represented in matrix form as

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \tag{1.1}$$

while in 3D the stress tensor is given by

$$\sigma_{ij} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \tag{1.2}$$

Here compressive stresses and forces are taken to be positive as this is the convention typically adopted in geomechanics (refer to Figure 1.10(a)). The components along the diagonal (σ_{xx}, σ_{yy}, σ_{zz}) are the *normal* or *direct* stresses, while the off-diagonal terms (σ_{xy}, σ_{yx}, σ_{zx}, etc.) are the shear stresses. When a material is

in a state of static equilibrium with equal complementary shear stresses, then the stress tensor is symmetric and we can say $\sigma_{ij} = \sigma_{ji}$. As illustrated in Figure 1.10 for every stress state (two- or three-dimensional) planes oriented at θ and $\theta + \frac{1}{2}\pi$ to the horizontal can be found in the material along which no shear stresses are felt. The direct stresses acting on these planes are called the principal stresses and the normals to the planes give the principal stress orientations. The principal stresses are given by the eigenvalues of the stress tensor, while the eigenvectors give the principal stress orientations. Typically the maximum or *major* principal stress is denoted by σ_1 and the minimum or *minor* principal stress is denoted by σ_3. In 3D there will also be an *intermediate* principal stress σ_2, with $\sigma_1 > \sigma_2 > \sigma_3$.

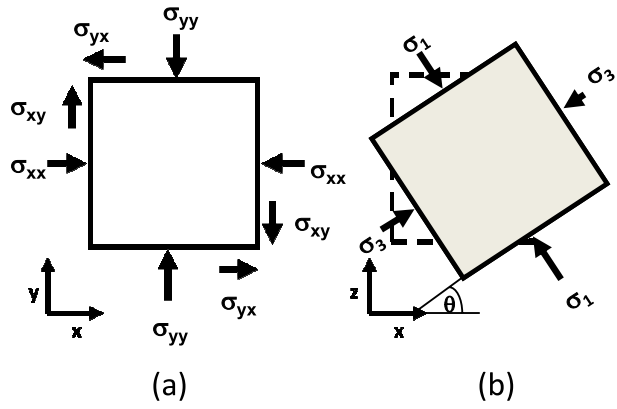


Figure 1.10: Illustration of two-dimensional stress state

The notation for addition and subtraction of vectors using tensors is straightforward. For example consider two contacting (touching) particles a and b. If the centroid of particle a has a position vector x_i^a and the centroid of particle b has a position vector x_i^b, then the vector giving the location of particle b relative

to particle a (called the branch vector) is given by $l_i = x_i^b - x_i^a$. In 3D this operation expands as follows:

$$l_i = \begin{pmatrix} l_x \\ l_y \\ l_z \end{pmatrix} = \begin{pmatrix} x_x^b - x_x^a \\ x_y^b - x_y^a \\ x_z^b - x_z^a \end{pmatrix} \tag{1.3}$$

As noted above, the tensorial notation system includes many ways for expressing mathematical operations involving vectors (1D arrays) and matrices concisely. The "dummy index" is used to indicate that we are considering terms along the diagonal, and less intuitively it denotes summation. Using this approach the trace of the stress tensor is given by σ_{ii}, and this is given by

$$\begin{array}{rcll} \sigma_{ii} & = & \sigma_{xx} + \sigma_{yy} & \text{(2D)} \\ \sigma_{ii} & = & \sigma_{xx} + \sigma_{yy} + \sigma_{zz} & \text{(3D)} \end{array} \tag{1.4}$$

The sum σ_{ii} is the first invariant of the stress tensor (I_σ). This parameter is "invariant" (i.e. unchanging) if the tensor is subject to an orthogonal rotation, e.g. if the tensor is rotated to consider the components along the principal axes of stress.

The dummy index concept can be extended to operations involving more than one tensor. For example, consider the contact force vector between two particles to be denoted by f_i and the branch vector to be denoted by l_i. In the expression $f_i l_i$, i is a dummy index and indicates reference to the inner product, i.e.

$$\begin{array}{rcll} f_i l_i & = & f_x l_x + f_y l_y & \text{(2D)} \\ f_i l_i & = & f_x l_x + f_y l_y + f_z l_z & \text{(3D)} \end{array} \tag{1.5}$$

In a similar manner, in three dimensions, the magnitude of a vector $|\mathbf{v}|$ is given by

$$|\ \mathbf{v}\ | = \sqrt{v_i v_i} = \sqrt{v_x v_x + v_y v_y + v_z v_z} \tag{1.6}$$

The use of free indices gives the expression $f_i l_j$ and this can be used to represent $f_x l_y$ when $i = x$ and $j = y$ or $f_x l_x$ when $i = x$ and $j = x$. Expressions similar to $\sum_N f_i l_j$ are used throughout

this book. The expansions of this expression in two and three dimensions are:

$$\begin{aligned} \sum_N f_i l_j &= \begin{pmatrix} \sum_N f_x l_x & \sum_N f_x l_y \\ \sum_N f_y l_x & \sum_N f_y l_y \end{pmatrix} \quad \text{(2D)} \\ \sum_N f_i l_j &= \begin{pmatrix} \sum_N f_x l_x & \sum_N f_x l_y & \sum_N f_x l_z \\ \sum_N f_y l_x & \sum_N f_y l_y & \sum_N f_y l_z \\ \sum_N f_z l_x & \sum_N f_z l_y & \sum_N f_z l_z \end{pmatrix} \quad \text{(3D)} \end{aligned} \tag{1.7}$$

Note that the product $f_i l_j$ is called the *dyadic* product of the two vectors $\mathbf{f}$ and $\mathbf{l}$, and this can also be expressed as $\mathbf{f} \otimes \mathbf{l}$.

In another example involving the use of the dummy index, the stress acting along a direction specified by the normal (unit) vector n_j can be calculated by multiplying the normal vector by the stress tensor. In tensorial notation this operation is expressed as $\sigma_{ij} n_j$. As above, repetition of the index j (the dummy index in this case) in the term $\sigma_{ij} n_j$ indicates that there will be a summation. The expansion (in 3D) is given by

$$\sigma_{ij} n_j = \sigma_{ix} n_x + \sigma_{iy} n_y + \sigma_{iz} n_z = \begin{pmatrix} \sigma_{xx} n_x + \sigma_{xy} n_y + \sigma_{xz} n_z \\ \sigma_{yx} n_x + \sigma_{yy} n_y + \sigma_{yz} n_z \\ \sigma_{zx} n_x + \sigma_{zy} n_y + \sigma_{zz} n_z \end{pmatrix} \tag{1.8}$$

Gradients are often of interest in geomechanics, and in the current context the use of a deformation gradient to calculate strain is important. Tensorial notation provides a concise notation for partial derivatives. In this case a comma, " , ", is used to indicate a partial derivative, i.e. the notation $v_{i,j}$ indicates the spatial partial derivative of the terms in vector v_i with respect to coordinate j. For example, if the vector describing the incremental displacement of a particle is given by u_i the displacement gradient is given by $u_{i,j}$ and in the 3D case this expands to

$$u_{i,j} = \begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} \end{pmatrix} \tag{1.9}$$

In addition to spatial derivatives we also need to consider temporal derivatives, i.e. rates. The notation $\dot{u}_i$ is used to denote the rate of change of the tensor u_i with respect to time, i.e.

$$\dot{u}_i = \begin{pmatrix} \frac{\partial u_x}{\partial t} \\ \frac{\partial u_y}{\partial t} \\ \frac{\partial u_z}{\partial t} \end{pmatrix} \tag{1.10}$$

Finally in relation to tensorial notation it is useful to introduce two specific tensors, the Kronecker delta δ_{ij} and the alternating tensor e_{ijk}. The Kronecker delta is defined to have the property

$$\delta_{ij} \quad = \quad \begin{cases} 1 & \text{when } i = j \\ \\ 0 & \text{when } i \neq j \end{cases} \tag{1.11}$$

The product of the Kronecker delta and a second-order tensor is given by

$$\sigma_{ij}\delta_{jk} = \sigma_{ik} \tag{1.12}$$

In this expression j is a dummy index and the free indices on each side of the equation are the same.

The alternating tensor is given by

- $e_{ijk} = 1$ when the indices are in the order xyz, yzx, zxy, i.e. cyclic order of indices.
- $e_{ijk} = -1$ when the indices are in the order xzy, yzx, zyx, i.e. anticyclic order of indices.
- $e_{ijk} = 0$ when there are repeated indices, e.g. xxy, xxz, xyy, etc.

The alternating tensor can be used to calculate the cross product of two tensors; in three dimensions the cross product is given by $\mathbf{c} = \mathbf{a} \times \mathbf{b}$ where

$$c_i = e_{ijk} a_j b_k \tag{1.13}$$

The vector $\mathbf{c}$ will be orthogonal to both $\mathbf{a}$ and $\mathbf{b}$.

1.7 Orthogonal Rotations

Chapters 2, 5 and 8 all refer to rotation of parameters. For example, when moving from a coordinate system defined by the principal axes of inertia of a given particle to the global coordinate system. To achieve this rotation an orthogonal rotation tensor is required. If a rotation is orthogonal then the product of two successive rotations is given by

$$T_{ij} T_{kj} = \delta_{ik} \tag{1.14}$$

Furthermore the transpose of $\mathbf{T}$ will equal the inverse of $\mathbf{T}$, $\mathbf{T}^T = \mathbf{T}^{-1}$. We can rotate any vector $\mathbf{a}$, with components (a_x, a_y, a_z) using a rotation tensor, using the tensor product $a'_i = T_{ij} a_j$ where the tensor a'_i gives the rotated components of the vector $\mathbf{a}$. The magnitude of the vector will remain unchanged, i.e. $|a_j| = |a'_i|$.

In three dimensions to rotate a vector a_i through an angle θ about the $z-$axis the following expression is used:

$$\begin{pmatrix} a'_x \\ a'_y \\ a'_z \end{pmatrix} = \mathbf{T} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \tag{1.15}$$

where a_i represents the original vector and a'_i is the rotated vector. When a vector is multiplied by an orthogonal rotation matrix a rigid body rotation is achieved, i.e. the vector length is preserved as the orientation changes.

While the basic DEM calculations are almost exclusively operations on one-dimensional vectors (i.e. particle velocity vector, contact force vector), analysis of the system typically involves the use

of second-order tensors (2D matrices), including the stress tensor, the strain tensor and the fabric tensor. To rotate a second-order tensor (σ_{ij}) from one coordinate system to another the operation is given by

$$\begin{pmatrix} \sigma'_{xx} & \sigma'_{xy} \\ \sigma'_{yx} & \sigma'_{yy} \end{pmatrix} = \mathbf{T} \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix} \mathbf{T}^T \tag{1.16}$$

1.8 Tessellation

The particulate systems considered in this book comprise discrete particles and their contacts. The creation of triangulations of the system is useful for applications including construction of the initial specimen geometry (Chapter 7), application of boundary stresses (Chapter 5), calculation of strain (Chapter 9), and analysis of the material fabric (Chapter 10). An overview of triangulation is therefore included at this point. More detailed considerations of the application of Delaunay triangulation in granular mechanics are given by Li and Li (2009), Goddard (2001), Ferrez (2001) and Bagi (1999a). Rapaport (2004) describes the implementation of a subroutine to construct a Voronoi polygon to analyse the structure of particulate systems in a molecular dynamics code, while Ferrez (2001) discusses the use of triangulation for contact detection. It may also be possible to use triangulation to couple DEM particle codes with continuum mechanics to represent a fluid phase.

A tessellation is a general term to describe the division of a space into a set of subspaces that do not overlap and that fill the space completely (i.e. with no gaps). These tessellations can exist in two- and three-dimensional space. Amongst the most commonly used tessellations are the Delaunay triangulation and the Voronoi diagram; these geometrical constructs are closely related and each is said to be the "dual" of the other. From a geomechanics perspective it is useful to realize that Delaunay triangulation is often used in mesh generation for finite element analyses of complex geometries.

Referring to Shewchuk (1999), for example, a triangulation of

a set of n points or nodes, $\mathbf{P} = \{P_1, P_k, P_n\}$, is a set of m ($m \neq n$) triangles, $\mathbf{T} = \{T_1, T_k, T_m\}$ whose interiors do not intersect each other. A Delaunay triangulation of a nodal set has the property that no node in the nodal set falls in the interior of the circumcircle (circle that passes through all three vertices) of any triangle in the triangulation. The Delaunay triangulation of the vertex set is unique. Higher-dimensional Delaunay triangulations are a generalization of the two-dimensional Delaunay triangulation. In three dimensions, the triangulation of V yields a set, T, of tetrahedra, whose vertices are V, and whose interiors do not intersect each other. In this case no node in the nodal set falls in the interior of the circumsphere (sphere that passes through all four vertices) of any tetrahedron in the triangulation. The Delaunay triangulation of 10 random points (nodes) in two dimensions is illustrated in Figure 1.11(b) and a three-dimensional triangulation is illustrated in Figure 1.12.

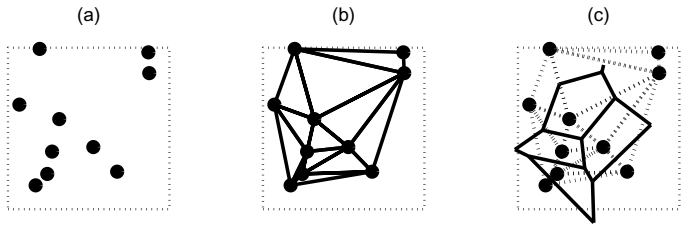


Figure 1.11: (a) 10 random points (b) Delaunay triangulation (c) Voronoi diagram

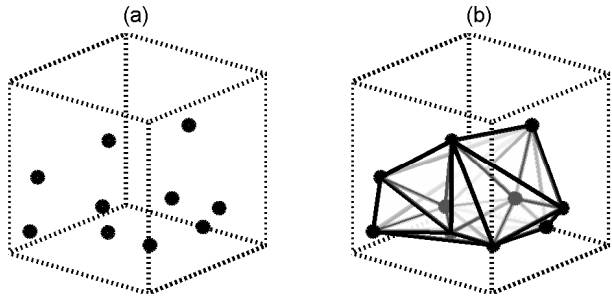


Figure 1.12: (a) 10 random points (b) Tetrahedra generated by 3D Delaunay triangulation

As discussed by Okabe et al. (2000), there are a number of different algorithms available for the implementation of Delaunay triangulation. Most of the triangulations used in this work were calculated using MATLAB, which uses the qhull algorithm (Barber et al., 1996).

As noted above, the Delaunay triangulation is related to (or is the dual of) a second geometrical construct called the Voronoi diagram or the Voronoi tessellation. The Voronoi diagram of a set of n nodes $\mathbf{P} = \{P_1, P_k, P_n\}$, is a set of n polygons, $\mathbf{V} = \{V_1, V_k, V_m\}$. Each polygon V_k is centred around a corresponding node P_k. The polygon V_k encloses an area or volume, such that every point within that polygon that is closer to the node P_k than to any other node in the set $\mathbf{P}$. The Voronoi diagram for the system of points given in Figure 1.11(a) is illustrated in Figure 1.11(c).

1.9 General Comments on Computer Modelling

A DEM model is an idealization of the real physical system and the extent of the idealizations used in creating the model will be discussed at various points in this text. It is important also to always be aware that a DEM simulation is a computer simulation and the

calculations are performed using finite, floating point representations of the real numbers, i.e. representations of the real numbers containing only a finite number of digits. An introduction to some of the issues associated with floating point arithmetic is given by Burden and Faires (1997) and a more detailed discussion is given by Goldberg (1991). The error associated with representing a real number in the floating point format used by computers is called a round-off error. The calculations in DEM simulations are therefore carried out on approximate representation of real numbers and the results of the calculations themselves are also subject to a round-off, which will introduce a further error into the system. One way to reduce round-off error is to reduce the number of error generating calculations. Care should also be taken in the choice of algorithm used to accurately resolve the contact geometry or the time integration approach. These issues are considered further in Chapter 4.

Chapter 2

Particle Motion

2.1 Introduction

A discrete element analysis is a dynamic or transient analysis that considers the dynamic interaction of a system of interacting particles. A particulate DEM model creates an ideal system of rigid particles that can move, connected by rigid springs that simulate the contact interactions. (The contact spring formulations are outlined in Chapter 3). As particles move away from each other contacts are broken and some of the springs will be removed; at the same time additional springs will be introduced as new contacts are formed. The continuous removal and introduction of contact springs results in a change in the overall system stiffness. A reduction in stiffness will also occur if a contact starts to slide. Therefore the analysis is non-linear. This non-linearity could be described as a geometrical non-linearity as it arises owing to a change in the local packing geometry of the particles. As will be discussed in Chapter 3, the contact constitutive model used to describe the force displacement response at the contacts is often non-linear, and this adds a material non-linearity to the system. These two particle-scale sources of non-linearity combine to give an overall non-linear macro-scale material response. At larger strains where sliding occurs the geometric non-linearity caused by gross movements at the contacts and "buckling" mechanisms that can develop in local groups of particles will dominate the response,

while the influence of the non-linear response at the contacts will be more evident at small strain levels, before the onset of sliding.

The basic principles of DEM are normally introduced by directly considering the dynamic equilibrium of the individual particles. Here DEM is introduced in a slightly different way. Civil engineers are usually familiar with the basic theories of matrix structural analysis and finite element analysis. In these approaches typically a large system of linear equations or stiffness matrix is formed. The displacements of the structural elements are determined by inverting this stiffness matrix. Particulate DEM uses a different solution strategy that introduces a greater risk of numerical instability (it is conditionally rather than unconditionally stable). To understand why the conditionally stable approach is preferred in particulate DEM, it is useful to initially consider DEM from the perspective of matrix structural analysis. As was already shown in Figure 1.4, the particles are analogous to the degrees of freedom in a matrix structural analysis (i.e. the end points of the structural elements) or alternatively the nodes in a finite element mesh. Using this analogy, the overall governing equation for the system can be expressed as the standard governing equation for a dynamic analysis in structures or continuum finite element or finite difference analysis, so that

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}(\mathbf{u}) = \Delta\mathbf{F} \tag{2.1}$$

where $\mathbf{M}$ is the mass matrix (or more correctly the inertia matrix , including both mass and rotational inertia), $\mathbf{C}$ is a damping matrix, $\mathbf{u}$ is the incremental displacement vector (including both translational and rotational displacements) and $\Delta\mathbf{F}$ is the incremental force vector (including moments). The global stiffness matrix $\mathbf{K}$ depends upon the system geometry, i.e. which particles are contacting. The incremental displacements are the movements of the particles over the current time step. The objective of the analysis is to solve for the incremental displacements. The velocity and acceleration vectors are given by $\dot{\mathbf{u}}$ and $\ddot{\mathbf{u}}$. The particles in a DEM model are then analagous to the nodes in a finite element analysis. However, as the particles are free to rotate, a particle in a 2D DEM analysis has three degrees of freedom (two translational

and one rotational), while a particle in a 3D DEM analysis has six degrees of freedom (three translational and three rotational).

Equation 2.1 is the dynamic equilibrium equation for the system. Broadly speaking, two approaches can be used to solve the dynamic equilibrium equation for a multi-nodal system. These approaches are termed *implicit* and *explicit*. In the implicit approach a single vector $\mathbf{u}$ can be created to represent the combined incremental displacements for all the particle centroids in the system. This is similar to the use of a single vector to represent the displacements of all the nodes in a finite element analysis, i.e.

$$\mathbf{u} = \begin{pmatrix} u_x^1 \\ u_y^1 \\ u_z^1 \\ u_x^p \\ u_y^p \\ u_z^p \\ u_x^{N_p} \\ u_y^{N_p} \\ u_z^{N_p} \end{pmatrix} \tag{2.2}$$

where u_x^p, u_y^p, u_z^p, are the incremental translational displacements of particle p in the three coordinate directions respectively and there are N_p particles in the system. (To simplify the discussion rotations are not considered at this point.) The incremental force vector $\Delta\mathbf{F}$ is constructed in a similar manner. The global mass $\mathbf{M}$, stiffness $\mathbf{K}$ and damping $\mathbf{C}$ matrices are combined as for the finite element method or in structural analysis. The global stiffness matrix construction is not detailed here and interested readers should refer to the finite element or structural analysis

texts of Zienkiewicz and Taylor (2000a) or Sack (1989) for guidance on stiffness matrix construction. Ke and Bray (1995) discuss the stiffness matrix formation for the implicitly particulate DEM algorithm DDAD (Discontinuous Deformation Analysis for Disks).

Where algorithms that involve assembly of a stiffness matrix are adopted to solve the dynamic equilibrium equation (Equation 2.33), a large system of simultaneous equations is generated, as in the finite element method, and solution will involve inversion of a highly sparse stiffness matrix. For a relatively small 3D system with 1,000 particles, the stiffness matrix will have 36×10^6 entries including the 0 valued terms as each particle has 6 degrees of freedom. Even if efficient algorithms to solve sparse systems of linear equations are used, the sequence of calculations will be very computationally expensive, both in terms of the number of operations required to solve the system and in terms of memory requirements. While some further consideration to this type of approach is given in Section 2.5 below, most geomechanics researchers use an alternative *explicit* approach that was originally outlined by Cundall and Strack (1979a,b).

In Cundall and Strack's distinct element approach, and in molecular dynamics, solution of the global system of equations is avoided by considering the dynamic equilibrium of the individual particles rather than solving the entire system simultaneously. This approach also avoids creation and storage of the large global stiffness matrix and, as highlighted by Potyondy and Cundall (2004), relatively modest amounts of computer memory are then required to consider large populations of particles. The implementation is somewhat similar to the implementation used for finite difference continuum analysis. Referring to Zhu et al. (2007) probably the most general format for expressing the equation governing the translational dynamic equilibrium of a particle p with mass m_p is

$$m_p \ddot{\mathbf{u}}_p = \sum_{c=1}^{N_{c,p}} \mathbf{F}_{pc}^{\text{con}} + \sum_{j=1}^{N_{nc,p}} \mathbf{F}_{pj}^{\text{non-con}} + \mathbf{F}_p^f + \mathbf{F}_p^g + \mathbf{F}_p^{\text{app}} \qquad (2.3)$$

where $\ddot{\mathbf{u}}_\mathbf{p}$ is the acceleration vector for particle p, $\mathbf{F}_{pc}^{\text{con}}$ are the con-

tact forces due to contact c when there are $N_{c,p}$ contacts between particle p and either other particles or boundaries, and $\mathbf{F}_{ck}^{\text{non-con}}$ are non-contact forces between particle p and $N_{nc,p}$ other particles (or boundaries). From a geomechanics perspective, the most likely origin of non-contact forces would be capillary forces in unsaturated soil. $\mathbf{F}_p^f$ is the fluid interaction force acting on particle p, $\mathbf{F}_p^g$ is the gravitational (body) force and $\mathbf{F}_p^{\text{app}}$ is a specified applied force (for example this may arise where a "stress-controlled membrane" is used as discussed in Section 5.4). Comparing Equations 2.1 and 2.3, there is no explicit consideration of damping in Equation 2.3, rather the contribution from damping is included in the calculation of the contact force (refer to the viscous dashpots described in Chapter 3 and also to Section 2.7 below).

The torque generated at each contact point is calculated as the cross-product of the contact force and a vector from the centre of the particle to the contact point. The dynamic rotational equilibrium is given by

$$\mathbf{I}_p \frac{d\boldsymbol{\omega}_p}{dt} = \sum_{j=1}^{N_{\text{mom}}} \mathbf{M}_{pj} \tag{2.4}$$

where $\boldsymbol{\omega}_p$ is the angular velocity vector and $\mathbf{M}_{pj}$ is the moment applied by the jth moment transmitting contact forces involving particle p and there are a total of N_{mom} moment transmitting contacts. As will be discussed in more detail in Chapter 3, at each contact point there will be a component of the contact force that is normal to the contact and a second component that acts along or tangential to the contact. The tangential forces will always impart a moment; however, the normal forces will only impart a moment if their line of action does not pass through the centroid of the particle (i.e. if the particles are non-circular or non-spherical). Moment transmitting contact models, e.g. rotational springs or the parallel bond model, have also been proposed.

During the deformation of a granular material the particle positions and the forces acting on the particles continuously evolve. In a DEM simulation time is discretized; this means that the system is examined at specific points in time and the real, continuously changing physical system is not accurately captured. As illus-

trated in Figure 1.8 in Chapter 1, at each time step there are two main sequences of calculations. The contact forces are calculated based on the most recently updated particle positions. This means that the applied forces and torques in Equations 2.3 and 2.4 are assumed to be known. Then Equations 2.3 and 2.4 can therefore easily be manipulated to give the particle translational and rotational accelerations, $\dot{\omega}_p$ and $\ddot{\mathbf{u}}_p$, i.e. equilibrium equations generate two sets of ordinary differential equations for each particle.

2.2 Updating Particle Positions

Knowing the resultant forces acting on the particles we can calculate the accelerations for particle p from the equation of dynamic equilibrium for the particle. If the translation motion of the particle is isolated, this equation is simply given by:

$$\mathbf{m}_p \mathbf{a}_p^t = \mathbf{F}_p^t \tag{2.5}$$

where $\mathbf{m}_p$ is the inertia (mass) matrix, $\mathbf{a}_p^t = \ddot{\mathbf{u}}_p^t$ is the acceleration vector at time t, and $\mathbf{F}^t$ is the resultant force vector. Note that the acceleration vector, $\mathbf{a}^t$ considers only the translational degrees of freedom and has 2 components in two dimensions and 3 components in three dimensions. The force vector $\mathbf{F}^t$ also has 2 components in two dimensions and 3 in three dimensions. In the two-dimensional case the mass (inertia) matrix is given by

$$\mathbf{m_p} = \begin{pmatrix} m_p & 0 \\ 0 & m_p \end{pmatrix} \tag{2.6}$$

where m_p is the particle mass, calculated as the particle density times the volume. In three dimensions the mass matrix, $\mathbf{m_p}$ is a 3×3 matrix, with the diagonal terms equal to m_p, and the off-diagonal terms equal to 0.

The next stage in the analysis involves using these acceleration values to obtain incremental displacements and hence update the particle positions. In numerical analysis, the techniques used to update parameters given their first and second derivatives with respect to time (i.e. to get displacements from accelerations),

are called time integration methods. Many time integration algorithms exist (reference to Wood (1990b) may be useful for readers specifically interested in this topic). It is important to appreciate that for general 3D particles, analysis of the rotational motion is significantly more complex than the translational motion.

In most DEM codes a time integration approach similar to the central-difference method with a time increment Δt is used. This approach can most easily be understood by considering the relationship between the acceleration and velocity vectors, as follows:

$$\mathbf{a}_p^t = \frac{1}{\Delta t}(\mathbf{v}_p^{t+\Delta t/2} - \mathbf{v}_p^{t-\Delta t/2}) \tag{2.7}$$

where $\mathbf{v}_p^{t-\Delta t/2}$ and $\mathbf{v}_p^{t+\Delta t/2}$ are the velocity vectors at $t - \Delta t/2$ and $t + \Delta t/2$ respectively for particle p. Rapaport (2004) terms this time integration approach a "leap-frog" method as the velocities and displacements are calculated with a time lag of $\Delta t/2$. Other authors (e.g. Munjiza (2004)) refer to it as the position Verlet time integration scheme. As with $\mathbf{F}_p$ and $\mathbf{a}_p$, the $\mathbf{v}_p$ vector has 3 components in two dimensions and 6 components in three dimensions. The velocity at time $t + \Delta t/2$ is then calculated as:

$$\mathbf{v}_p^{t+\Delta t/2} = \mathbf{v}_p^{t-\Delta t/2} + \Delta t \mathbf{m}_p^{-1}(\mathbf{F}_p^t) \tag{2.8}$$

The velocity at time $t + \Delta t/2$ is taken to equal the average velocity over the time increment t to $t+\Delta t$. Then we can calculate the updated particle position $\mathbf{d}_p^{t+\Delta t}$ as:

$$\mathbf{x}_p^{t+\Delta t} = \mathbf{x}_p^t + \Delta t \times \mathbf{v}_p^{t+\Delta t/2} \tag{2.9}$$

where the particle position vector $\mathbf{x}$ gives the particle Cartesian coordinates and the total rotation about the principal axis (axes in 3D).

For two-dimensional discrete element simulations there is no coupling between the three degrees rotational of freedom. This means that the particle's rotational or angular velocities can be calculated by considering the following dynamic rotational equilibrium equation:

$$I_{p,z}\dot{\omega}_{p,z} = M_{p,z} \tag{2.10}$$

where $\omega_{p,z}$ is the angular velocity about an axis through the centre of the particle orthogonal to the analysis plane. For a circular or disk particle the moment of inertia $I_{p,z}$ equals $\frac{\rho\pi r_p^4}{2}$ where r_p is the particle radius and ρ is the particle density. The central-difference time integration approach can easily be applied to incrementally solve this equation as follows:

$$\omega_{p,z}^{t+\Delta t/2} = \omega_{p,z}^{t-\Delta t/2} + \Delta t \frac{M_{p,z}^{t}}{I_{p,z}} \tag{2.11}$$

This angular velocity is used to calculate the tangential component of the contact force (refer to Section 3.7). It is also used to update the position of the edges of non-spherical particles, and to calculate the total particle rotations (rotations are important as an indicator of localizations within the material (Chapter 8). A key decision to be made by the analyst is to choose the value of the time increment, Δt, to be used in the simulation.

2.3 Time integration and Discrete Element Modelling: Accuracy and Stability

In their description of the distinct element method Cundall and Strack (1979a) proposed the use of the computationally efficient, explicit, central-difference type time integration scheme. A limitation of this scheme is that it is only conditionally stable, so small time steps must be used. However, this restriction on the size of the time increment due to numerical stability considerations is not as limiting as it might initially appear. To successfully capture the inherent non-linearity of the problem (changing contact conditions and non-linear contact response) the incremental changes in the particle positions and contact forces in a given time-step must be small. This translates into a constraint on the time increment to be small to capture the non-linearity of the system. Ideally the time increment chosen in a DEM simulation should be small enough that the motion of a particle over a given time step

is sufficiently small to only influence its immediate neighbouring particles. Cundall and Strack (1978) stated that a fundamental idea of DEM is that the time step chosen be sufficiently small that in a single time step disturbances cannot propagate from a disk further than its nearest neighbours.

In the context of analysis of physical systems, a numerical algorithm is a procedure involving a sequence of calculations developed to model the response of the system. In DEM there is a set of calculations where information about the current configuration of particles is used to step forward and predict the system state at a future time. This prediction will be approximate, rather than exact. It is important to carefully consider the limitations and approximations involved in the numerical model. In DEM it is important to consider the accuracy, stability and robustness of the time integration algorithm used. Sutmann (2002) considers these issues from a molecular dynamics perspective. During each cycle in a DEM simulation the dynamic equilibrium equation is solved for each particle in the assembly. The system of differential equations is an idealization of the real physical system, limiting accurate prediction. Specific approximation errors are introduced when the equation is solved numerically. The round-off error introduced in calculations using computers is considered briefly in Section 1.9. A second, much larger, error is introduced as a consequence of the approximations used to calculate the particle incremental displacements from the calculated accelerations. This error is called the truncation error.

In any numerical model that simulates the response of a transient or dynamic system there will be truncation errors introduced at each time step. The truncation error can be understood by reference to the Taylor series expansion. The Taylor series expansion provides an estimate for the value of a parameter, say the position, at time $t + \Delta t$ as given by $\mathbf{x}_{t+\Delta t}$, in terms of the position at time t and the temporal derivatives of the position at time t, as

$$\mathbf{x}_p^{t+\Delta t} = \mathbf{x}_p^t + \Delta t \left(\frac{d\mathbf{x}_p}{dt} \right)^t + \frac{\Delta t^2}{2!} \left(\frac{d^2\mathbf{x}_p}{dt^2} \right)^t + \frac{\Delta t^n}{n!} \left(\frac{d^n\mathbf{x}_p}{dt^n} \right)^t + O\left(\Delta t^{n+1}\right) \tag{2.12}$$

The term $O(\Delta t^{n+1})$ is the truncation error. This is the error introduced in the approximate, calculated value of $\mathbf{x}_p^{t+\Delta t}$ by considering only the first n derivatives of $\mathbf{x}_p$ at time t in the prediction. This truncation error is a measure of the amount by which the exact solution to the differential equation describing the particle motion differs from the approximate solution. The error is proportional to Δt^{n+1}. As Δt will be a small number, i.e. $\Delta t << 1$, then the higher the value of n, and hence the greater the number of derivatives that are included in the approximation, the smaller the error will be. The error will also be reduced using a smaller Δt value, with the resultant improvement in accuracy being much greater for large values of n. In a transient simulation, where we are calculating the values of $\mathbf{x}_t$ over many time increments, this error is considered to be a "local" truncation error that is introduced at each time increment.

Most DEM codes used in geomechanics use either the central-difference time integration algorithm or a slightly modified version of the central-difference method. As noted by Wood (1990b) there is more than one expression available for the central-difference time integration approach. The Verlet equations used in DEM are given by

$$\begin{aligned} \mathbf{v}_p^{t+\Delta t/2} &= \mathbf{v}_p^{t-\Delta t/2} + \Delta t \mathbf{a}_p^t \\ \mathbf{x}_p^{t+\Delta t} &= \mathbf{x}_p^t + \Delta t \mathbf{v}_p^{t+\Delta t/2} \end{aligned} \tag{2.13}$$

In an alternative form of the central-difference method, the incremental displacement is calculated directly from the particle accelerations at time t (Wood, 1990b), so that

$$\Delta \mathbf{x}_p^{t \to t+\Delta t} = \Delta \mathbf{x}_p^{t-\Delta t \to t} + \Delta t^2 \mathbf{a}_p^t \tag{2.14}$$

where $\Delta \mathbf{x}_p^{t \to t+\Delta t}$ is the incremental displacement over the time increment from t to $t + \Delta t$, i.e. $\Delta \mathbf{x}^{t \to t+\Delta t} = \mathbf{x}_p^{t+\Delta t} - \mathbf{x}_p^t$ and $\Delta \mathbf{x}_p^{t-\Delta t \to t} = \mathbf{x}_p^t - \mathbf{x}_p^{t-\Delta t}$. This means that Equation 2.14 gives the acceleration as

$$\mathbf{a}_p^t = \frac{\left(\mathbf{x}_p^{t+\Delta t} - 2\Delta \mathbf{x}_p^t + \Delta \mathbf{x}_p^{t-\Delta t}\right)}{\Delta t^2} \tag{2.15}$$

In either form, the central-difference algorithm is a second-order scheme, i.e. the accuracy of the calculated displacement depends on the square of the time increment, Δt^2. This time integration scheme has also been implemented for consideration of structural dynamics problems, and reference to Chopra (1995) may be useful to aid in developing an understanding of this method. One author who discusses the issue of accuracy arising from the truncation error explicitly is Cleary (2000) who stated that for this method between 20 and 50 time increments are needed to accurately resolve each collision in his simulations, resulting in very small time increments.

When choosing a method to integrate the particle accelerations and calculate the updated particle coordinates, it is important that the method chosen be both *consistent* and *convergent*. If the local truncation error at step i is τ, then the method is consistent if $\lim_{\Delta t \to 0} |\tau| = 0$ for all steps in the calculation sequence. A method is convergent if $\lim_{\Delta t \to 0} |\mathbf{x}^{\text{exact},t} - \mathbf{x}^t| = 0$ where $\mathbf{x}^{\text{exact},t}$ is the exact solution to the differential equation describing the particle motion at time t, and x^t is the calculated (approximate) value at the same time. The truncation error will be magnified as the analysis proceeds, so at time $t = n\Delta t$ the error will be magnified n times.

The algorithm must also be "stable." There are a number of ways of explaining what is meant by "stability" in the context of numerical modelling. In general, for a stable system if there are small changes in the initial data input to the model, the resultant changes in the output will also be small. If an error, E_0, is introduced at a given point in time, the error after n subsequent calculations, E_n, is the global error. As noted by Burden and Faires (1997) it is difficult to determine the global error, but there is a close correlation between the local error and the global error. Typically a linear growth in the global error will be unavoidable, meaning that if a local error E_0 is introduced at some point in the calculation, the cumulative effect of the error after n time increments is $E_n = CnE_0$, where C is a constant. If the relationship between the local and global truncation errors is $E_n = CnE_0$ then the algorithm is typically stable, however if $E_n = C^nE_0$ where $n > 1$, then there will be an exponential growth in error and the

method is considered to be unstable. In mechanics applications analysts sometimes monitor the stability of a numerical model by calculating the total energy of the system. The components of the total energy include the strain energy stored in the contact springs and the particles' kinetic energy (refer to Section 2.6). Where the numerical integration is stable there will be no drift in the energy of the system. In an unstable system there will be a non-physical increase in energy in the system, i.e. energy is not conserved.

2.4 Stability of Central Difference Time Integration

The stability of the central-difference time integration approach is outlined in many basic numerical analysis texts (e.g. Burden and Faires (1997)). The basic idea of any time integration is that knowing the position and acceleration of a body we can predict its future displacement. Typically in numerical analysis/dynamics courses the concept is introduced by considering the free vibration of a particle of mass, m, suspended on a simple, elastic sphere with stiffness k. The dynamic equilibrium equation for this single degree of freedom system is then given by $a = -kx$, where $a = \ddot{x}$. For this simple system, if the central-difference approach is used, the maximum time increment that can be used is $\Delta t = \frac{T}{\pi}$, where T is the period for free oscillation of the system. This period is calculated as $T = 2\pi\sqrt{\frac{m}{k}}$. If predictions are made using a time increment that exceeds this critical value the results quickly become physically unreasonable and the analysis is said to be unstable. These restrictions on the choice of time increment that occur when using the central-difference approach to this simple, single degree of freedom system also apply in the multi degree of freedom simulations in DEM.

The critical time increment for stable analysis can be calculated using linear stability analysis by considering the *amplification matrix*, Zienkiewicz and Taylor (2000a). In general the amplification matrix, $\mathbf{A}$, is defined such that $\mathbf{x}_{t+\Delta t} = \mathbf{A}\mathbf{x}_t$. If any eigenvalue μ_i of $\mathbf{A}$ has a magnitude exceeding 1 (i.e. if $|\mu_i| > 1$) any initially

small errors will increase without bound and the analysis will be unstable. Note that the spectral radius of $\mathbf{A}$, $\rho(\mathbf{A})$, is the maximum magnitude of an eigenvalue of $\mathbf{A}$, i.e. $\rho(\mathbf{A}) = max\left(|\mu_i|\right)$ Munjiza (2004) adopts a slightly different approach and defines an amplification matrix $\mathbf{A}^*$ for a single degree of freedom system with position x so that

$$\begin{pmatrix} \dot{x}_{t+\Delta t}\Delta t \\ x_{t+\Delta t} \end{pmatrix} = \begin{pmatrix} 1 & -\frac{\Delta t^2 k}{m} \\ 1 & 1-\frac{\Delta t^2 k}{m} \end{pmatrix} \begin{pmatrix} \dot{x}_t \Delta t \\ x_t \end{pmatrix} = \mathbf{A}^* \begin{pmatrix} \dot{x}_t \Delta t \\ x_t \end{pmatrix} \tag{2.16}$$

Munijza shows that where $\frac{\Delta t^2 k}{m} \leq 4$ the spectral radius of $\mathbf{A}^*$, $\rho(\mathbf{A}^*)$ will be 1, however once $\frac{\Delta t^2 k}{m} > 4$ the spectral radius will increase beyond 1 and the simulation of the single degree of freedom system will be unstable. Stability analyses are completed by considering the undamped dynamic equilibrium equation, as is the case here. Wood (1990b) states that for simple algorithms, this assumption is valid.

Accepting this limitation of the central-difference method, it is necessary to examine the implications of the stability limitation for the multi degree of freedom systems encountered in DEM analyses. A DEM system is significantly more complex than the simple, single degree of freedom system. Each particle will have multiple contacts and multiple contact springs. At each contact there are two orthogonal springs acting normal and tangential to the contact. There will also most likely be a range of particle inertia values. O'Sullivan and Bray (2003b) proposed an approach to calculate a bound on the critical time increment for DEM simulations by drawing an analogy between a discrete element framework, and a finite element framework. In their analysis, the discrete element particles correspond to finite element nodes and that the inter-particle contacts correspond to the finite elements, as illustrated in Figure 2.1. A global stiffness matrix can be assembled as in a finite element analysis, with the contact between particle i and particle j forming an "element" stiffness matrix, $\mathbf{K}^e_{ij}$ and the mass matrix including the inertia of the particles. Itasca (2008) give an alternative derivation for the stiffness at a contact point that also accounts for translational and rotational motion.