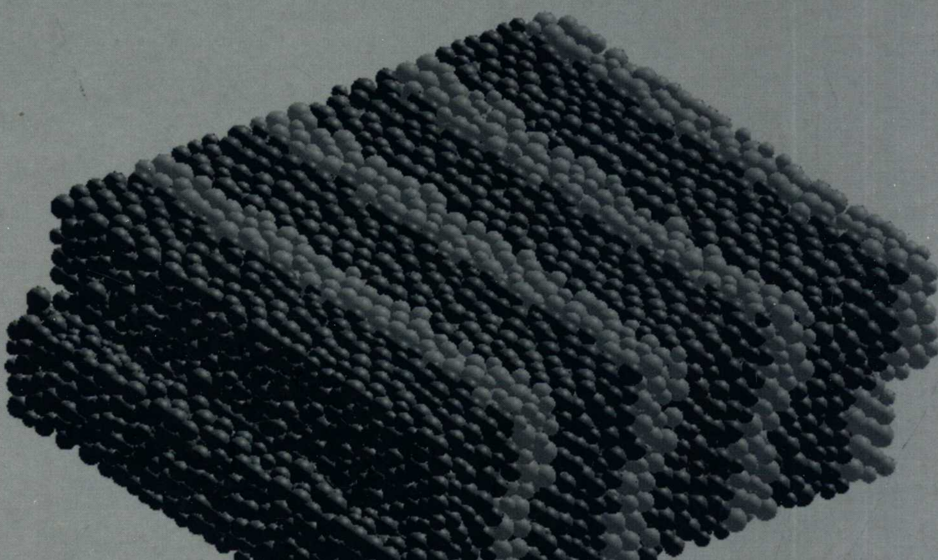
PARTICULATE DISCRETE ELEMENT MODELLING

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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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 discussions 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.

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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.

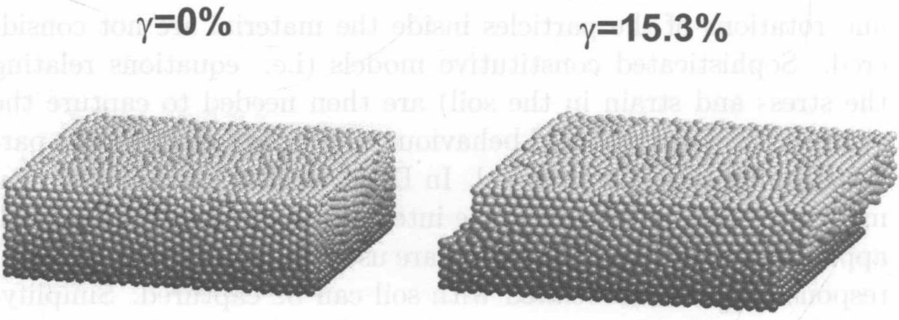

Figure 1.1: Simulation of a direct shear test using DEM

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 failure 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.

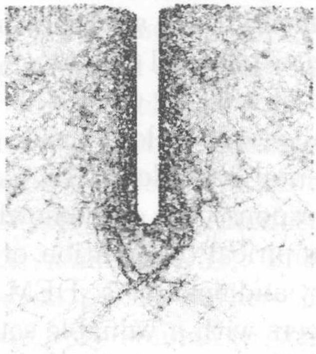

Figure 1.2: Two-dimensional DEM simulation of cone penetrometer penetrating a granular material (disk shading indicates magnitude of rotation)

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

