The Combined Finite-Discrete Element Method

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To Jasna and Boney
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Preface

Computational mechanics of discontinua is a relatively new discipline of computational mechanics. It deals with numerical solutions to engineering problems and processes where constitutive laws are not available. Particle-based modelling of micro-structural elements of material is used instead. Thus, the interaction and individual behaviour of millions, even billions, of particles is considered to arrive at emergent physical properties of practical importance.

Methods of computational mechanics of discontinua include DEM (Discrete Element Methods), DDA (Discontinua Deformation Analysis Methods), Methods of Molecular Dynamics, etc.

In the last decade of the 20th century, the Discrete Element Method has been coupled with the Finite Element Method. The new method is termed the ‘Combined Finite-Discrete Element Method’. Thanks to the relatively inexpensive high performance hardware rapidly becoming available, it is possible to consider combined finite-discrete element systems comprising millions of particles, and most recently even billions of particles. These, coupled with recent algorithmic developments, have resulted in the combined finite-discrete element method being applied to a diversity of engineering and scientific problems, ranging from powder technology, ceramics, composite materials, rock blasting, mining, demolition, blasts and impacts in a defence context, through to geological and environmental applications.

Broadly speaking, the combined finite-discrete element method is applicable to any problem of solid mechanics where failure, fracture, fragmentation, collapse or other type of extensive material damage is expected.

In the early 1990s, the combined finite-discrete element method was mostly an academic subject. In the last ten years, the first commercial codes have been developed, and many commercial finite element packages are increasingly adopting the combined finite-discrete element method. The same is valid for the commercial discrete element packages. The combined finite-discrete element method has become available to research students, but also to engineers and researchers in industry. It is also becoming an integral part of many undergraduate and postgraduate programs.

A book on the combined finite-discrete element method is long overdue. This book aims to help all those who need to learn more about the combined finite-discrete element method.
Acknowledgements

This book could not have happened without the support and encouragements of the publishers, Wiley, and many of my colleagues. I would like first to mention Professor J.R. Williams from MIT. He has always been an inspiration and a motivator, and ready to help throughout. I started my PhD under his guidance, and finished it while working in his laboratory at MIT. He was a great teacher then, just as he is today. He is one of those professors well remembered by students. I also owe a great deal to many others. This book could not have happened without the support from Dr. D.S. Preece, Prof. G. Mustoe, Dr. C. Thornton, Dr. J.P. Latham, Prof. D.R.J. Owen, Prof. B. Mohanty, Prof. E. Hinton, Prof. O. Zienkiewicz, Dr. K.R.F. Andrews, Prof. J. White, Dr. N. John, Prof. R. O’Connor, Prof. F. Aliabadi, Prof. Mihanovic, Prof. Jovic, and many others from whom I have learned. You have been real friends. Thank you.
1

Introduction

1.1 GENERAL FORMULATION OF CONTINUUM PROBLEMS

The microstructure of engineering materials is discontinuous. However, for a large proportion of engineering problems it is not necessary to take into account the discontinuous nature of the material. This is because engineering problems take material in quantities large enough so that the microstructure of the material can be described by averaged material properties, which are continuous. The continuous nature of such material properties is best illustrated by mass \( m \), which is defined as a continuous function of volume through introduction of density \( \rho \) such that

\[
\rho = \frac{dm}{dV}
\]

where \( V \) is volume. The microscopic discontinuous distribution of mass in space is thus replaced by hypothetical macroscopic continuous mass distribution. In other words, microscopic discontinuous material is replaced by macroscopic continuum of density \( \rho \).

The continuum hypothesis introduced is valid as long as the characteristic length of the particular engineering problem is, for instance, much greater than the mean free path of molecules. For engineering problems the characteristic length is defined by either the smallest dimension of the problem itself, or the smallest dimension of the part of the problem of practical interest. The hypothesis of continuum enables the definition of physical properties of the material as continuous functions of volume. These physical properties are very often called physical equations, or the constitutive law, and they are then combined with balance principles (balance equations). The result is a set of governing equations. The balance principles are \textit{a priori} physical principles describing materials in sufficient bulk so that the effects of discontinuous microstructure can be neglected. Balance principles include conservation of mass, conservation of energy, preservation of momentum balance, preservation of moment of momentum balance, etc.

Governing equations are usually given as a set of partial differential equations (strong formulation) or integral equations (weak or variational formulation). Governing equations, when coupled with external actions in the form of boundary and initial conditions (such as loads, supports, initial velocity, etc.), make a boundary value problem or an initial boundary value problem. The solution of a particular boundary value problem is sometimes expressed in analytical form. More often, approximate numerical methods are employed.
These include the finite difference method, finite volume method, finite element method, mesh-less finite element methods, etc.

The most advanced and the most often used method is the finite element method. The finite element method is based on discretisation of the domain into finite sub-domains, also called finite elements. Finite elements share nodes, edges and surfaces, all of which comprise a finite element mesh. The solution over individual finite elements is sought in an approximate form using shape (base) functions. Balanced principles are imposed in averaged (integral or weak) form. These usually yield algebraic equations, for instance equilibrium of nodal forces, thus effectively replacing governing partial differential equations with a system of simultaneous algebraic equations, the solution of which gives results (e.g. displacements) at the nodes of finite elements.

1.2 GENERAL FORMULATION OF DISCONTINUUM PROBLEMS

Taking into account that the mean free path of molecules for most engineering materials is very small in comparison to the characteristic length of most of the engineering problems, one may arrive at the conclusion that most engineering materials are well represented by a hypothetical continuum model. That this is not the case is easily demonstrated by the following problem:

A glass container of square base is filled with particles of varying shape and size, as shown in Figure 1.1. The particulate is left to fall from the given height. During the fall under gravity, the particles interact with each other and with the walls of the container. In this process energy is dissipated, and finally, all the particles find state of rest. The

Figure 1.1 Letting particles of different shape and size pack under gravity inside the glass container. The question is how much space will they occupy?
question is, what is the total volume occupied by the particulate after all the particles have found the state of rest?

This problem is subsequently referred to as container problem. It is self-evident that the definition of density $\rho$ given by

$$\rho = \frac{dm}{dV} \quad (1.2)$$

and the definition of mass $m$ given by

$$m = \int V \rho dV \quad (1.3)$$

are not valid for the container problem.

The total mass of the system is instead given by

$$m = \sum_{i=1}^{N} m_i \quad (1.4)$$

where $N$ is the total number of particles in the container and $m_i$ is the mass of the individual particles. In other words, the total mass is given as a sum of the masses of individual particles. It is worth mentioning that the size of the container is not much larger than the size of the individual particles. The particles pack in the container, and the mass of particles in the container is a function of the size of the container, the shape of individual particles, size of individual particles, deposition method, deposition sequence, etc.

Mathematical description of the container problem ought to take into account the shape, size and mass of individual particles, and also the interaction between the individual particles and interaction with the walls of the container. The mathematical model describing the problem has to state the interaction law for each couple of contacting particles. For each particle, the interaction law is combined with a momentum balance principle, resulting in a set of governing equations describing that particle. Sets of differential equations for different particles are coupled through inter-particle interaction. The resulting global set of coupled differential equations describes the behaviour of the particulate system as a whole. The solution of the global set of governing equations results in the final state of rest for each of the particles. In the case of hypothetical continuum the total number of governing partial differential equations does not depend on the size of the problem. In the container problem, each particle has a set of differential equations governing its motion, and the total number of governing partial differential equations is proportional to the total number of particles in the container.

The container problem, together with many similar problems pervading science and engineering, are by nature discontinuous. They are called problems of discontinuum, or discontinuum problems. Problems for which a hypothetical continuum model is valid are, in contrast, called problems of continuum, or continuum problems. The mathematical formulation of problems of continuum involves the constitutive law, balance principles, boundary conditions and/or initial conditions.

The mathematical formulation of problems of discontinua involves the interaction law between particles and balance principles. Analytical solutions of these equations are rarely available, and approximate numerical solutions are sought instead. The most advanced
and most often used numerical methods are Discontinuous Deformation Analysis (DDA) and Discrete Element Methods (DEM). These methods are designed to handle contact situations for a large number of irregular particles. DDA is more suitable for static problems, while DEM is more suitable for problems involving transient dynamics until the state of rest or steady state is achieved.

A division of computational mechanics dealing with computational solutions to the problems of discontinua is called Computational Mechanics of Discontinua. Computational Mechanics of Discontinua is a relatively new discipline. Pioneering work in the late 1960s and early 1970s was done by researchers (Williams, Cundal, Gen-She, Musto, Preece, Thornton) from various disciplines. They handled complex problems of discontinua with very modest computing hardware resources available at the time. A second generation of researchers, such as Munjiza, Owen and O’Connor, benefited not only from more sophisticated computer hardware, available with RAM space measured in megabytes, but also from the UNIX operating system and graphics libraries combined with a new generation of computer languages, such as C and C++. This has enabled the key algorithmic solutions to be developed and/or improved. The third generation of researchers (late 1990s and the early years of this century) has benefited further from increased RAM space, now measured in gigabytes, relatively inexpensive CPU power, sophisticated visualisation tools, the internet and public domain software. As a result of this progress, discontinua methods have been applied to a wide range of engineering problems, which include both industrial and scientific applications.

1.3 A TYPICAL PROBLEM OF COMPUTATIONAL MECHANICS OF DISCONTINUA

The difference between problems of Computational Mechanics of Continua and problems of Computational Mechanics of Discontinua are best illustrated by the container problem. The container problem is about how many particles can be placed in a given volume, how they interact and the mechanics of the pack in general. To demonstrate the key elements of discontinua analysis, a numerical simulation of gravitational deposition of different packs inside a rigid box of size 250 × 250 × 540 mm is shown in this section. The total solid volume deposited is constant for all simulations shown, and is equal to $V = 9.150e-03 \text{ m}^3$.

The particles are deposited in three stages:

- In the first stage, a regular pattern is used to initially place all the particles inside the box, (Figure 1.2 (left)).
- In the second stage, random velocity field is applied to all the particles, making particles move inside the box until a near random distribution of particles inside the box is achieved. There is no gravity at this stage (Figure 1.2 (right)).
- In the third stage, the velocity of all particles is set to zero, and acceleration of gravity $g = 9.81 \text{ m/s}^2$ is applied in the z-direction. Under gravity the particles move towards the bottom of the box. Due to the interaction with the box and with each other, the particles closer to the bottom of the box slowly settle into the final
position. Due to energy dissipation, eventually the velocity of all particles is zero and the pack is at the state of rest – which is also the state of static equilibrium. Thus, through dynamic governing equations taking into account dynamic equilibrium and through contact and the motion of individual particles, static equilibrium of the pack is achieved.

In Figures 1.2–1.6, such deposition sequence of a pack comprising identical spheres of diameter $d = 2.635$ mm is shown. As explained earlier, the total volume of the solid deposited is $V = 9.150e-03$ m$^3$. Thus, the pack comprises 955,160 identical spheres.

The maximum theoretical density for packs comprised of identical spheres is given by

$$
\rho = \frac{\pi \sqrt{18}}{18} \approx 0.7405
$$

A density profile obtained using gravitational deposition is normalised using this theoretical density. Density profiles for different packs are shown in Figure 1.7. Initially (solid line), the particles are almost uniformly distributed over the box; the density is only slightly larger at the bottom of the box than at the top.

The motion of the particles under gravity gradually increases density at the bottom of the pack and decreases density at the top of the pack, making the upper parts of the box empty. As the particles settle, the pack gets denser. At the state of rest (dashed line), almost uniform density over most of the pack is achieved, with rapid density decrease towards the top of the pack.
**Figure 1.3** Deposition sequence at 0.55 s (left) and 0.105 s (right).

**Figure 1.4** Deposition sequence at 0.155 s (left) and 0.180 s (right).
Figure 1.5  Deposition sequence at 0.230 s (left) and 0.255 s (right).

Figure 1.6  Deposition sequence at 0.605 s (left) and 0.830 s (right).
The final packing density achieved is smaller than the theoretical density. The reasons behind this can be investigated if the same volume of solid is deposited using identical spheres of a larger diameter. Thus, in Figures 1.8–1.13, numerical simulation of gravitational deposition of 139,968 spheres all of the same diameter \(d = 4.998\) mm is performed. The total solid volume of the spheres is the same as in the previous example, i.e. \(V = 9.150 \times 10^{-3} \text{ m}^3\).
Figure 1.9  Gravity induced motion of the pack after 0.055 s and 0.105 s.

Figure 1.10  Gravity induced motion of the pack after 0.155 s and 0.205 s.
Figure 1.11  Gravity induced motion of the pack after 0.255 s and 0.305 s.

Figure 1.12  Gravity induced motion of the pack after 0.405 s and 0.430 s.
Density profiles for this pack are shown in Figure 1.14. The density profiles shown are normalised using the theoretical density. Initially (solid line), the particles are loosely packed inside the box. The motion of the particles under gravity gradually increases density at the bottom of the pack and decreases density at the top of the pack, finally making the upper parts of the box empty. As the particles settle, the pack gets denser. At the state of rest (top line), almost uniform density over most of the pack is achieved,
with rapid density decrease towards the top of the pack. The final density is almost 10% smaller than the theoretical density for the same problem with periodic boundaries.

A further demonstration of the influence of sphere size on packing density is obtained through deposition of the same volume of solid, but comprised of larger spheres. Numerical experiments included:

- **41472 spheres of** $d = 7.497$ mm (Figure 1.15)
- **5184 spheres of** $d = 14.994$ mm (Figure 1.15)
- **648 spheres of** $d = 29.988$ mm (Figure 1.16)
- **192 spheres of** $d = 44.9829$ mm (Figure 1.16)
- **81 spheres of** $d = 59.976$ mm (Figure 1.17)
- **50 spheres of** $d = 70.439$ mm (Figure 1.17).

The final density profiles for each of the packs are given in Figure 1.18. The density of packs comprising very large spheres is very far from the theoretical density. This is due to the influence of the boundary conditions. For large spheres, the box is simply too small, and theoretical packing cannot be achieved.

As the spheres get smaller, the influence of the box diminishes and the density gets closer to the theoretical density, as shown in Figure 1.19, where packing density as a function of normalised sphere diameter (sphere diameter divided by the size of the edge of the box base—250 mm) is plotted. For large spheres the density can go either up or down with a reduction in sphere size, i.e. discontinuum behaviour is strongly pronounced. As the spheres get smaller, more uniform convergence toward the theoretical result is achieved. Thus, at zero sphere diameter, theoretical density is achieved.

![Figure 1.15](image-url) Final pack of spheres: left $d = 7.497$ mm, right $d = 14.994$ mm.
Figure 1.16 Final pack of spheres: left $d = 29.988$ mm, right $d = 44.982$ mm.

Figure 1.17 Final pack of spheres: left $d = 59.976$ mm, right $d = 70.439$ mm.
Figure 1.18 Final density profiles for selected diameters of spheres.

Figure 1.19 Maximum density as function of diameter of sphere and size of the box.

The container problem is a typical problem where continuum-based models cannot be applied. This problem also demonstrates that discontinuum-based simulations recover continuum formulation when the size of individual discrete elements (the diameter of the sphere in the problem described above) becomes small in comparison with the characteristic length of the problem being analysed. In the problem shown, the characteristic length of the problem is the length of the smallest edge of the box. The continuum-based models are simply a subset of more general discontinuum-based formulations; applicable when microstructural elements of the matter comprising the problem are very small in comparison to the characteristic length of the problem being analysed.

The behaviour of discontinuum systems is a function of the properties of microstructural elements (particles or discrete elements) making the system. The size of discrete