1

Introduction to Mechanics of Discontinua

1.1 The Concept of Discontinua

It was Galileo who noticed that the velocity of a free falling body increases by a constant amount in a given fixed increment of time. The more general case of this is the variable change of velocity, as shown in Figure 1.1. This velocity change can be written as

\[ a = \frac{\Delta v}{\Delta t} \]  

(1.1)

where \( a \) is the acceleration. From his observations one can say that Galileo nearly discovered differential calculus. The discovery of differential calculus would have naturally led him to the laws of motion and the story of classical mechanics would have come much earlier in history.

In reality it was Newton who extrapolated the concept of

\[ a = \lim_{\Delta t \to 0} \frac{\Delta v}{\Delta t} \]  

(1.2)

to the case that when \( \Delta t \) is nearly zero, instantaneous acceleration is achieved, as shown in Figure 1.2.

Leibnitz took the concept even further and generalized it, thus developing what is now called “differential calculus”. One could argue that differential calculus is the most important discovery of modern science. It has enabled scientists and engineers to describe physical problems in terms of governing equations. The governing equations are usually a set of partial differential equations that describe a particular engineering or scientific problem. Examples of these include equilibrium equations of the linear theory of elasticity and also the Navier-Stokes equations describing the flow of Newtonian fluids.

All of these are based on the concept of instantaneous, point or distributed quantity such as

\[ v = \frac{d\mathbf{r}}{dt} \]  

(1.3)
which is the instantaneous velocity or

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

(1.4)

which is the point density. Without differential calculus one would have to use the average density given by

\[ \bar{\rho} = \frac{\Delta m}{\Delta V} \]  

(1.5)

where \( \Delta V \) is some finite volume and \( \Delta m \) is the mass of that volume.

This concept can be expanded to any distributed quantity such as load

\[ p = \lim_{\Delta x \to 0} \frac{\Delta f}{\Delta x} \]  

(1.6)

where \( p \) is the value of the distributed load at a specific point, as shown in Figure 1.3.

Of course, in these extrapolations a hidden assumption is made: Qualitatively nothing changes as \( \Delta x \) or \( \Delta V \) gets smaller and smaller. This is the standard continuum assumption and it is both true and not true. It is true if one is solving a problem where one is really interested in results in terms of average quantities, that is, the physics of the problem are contained at relatively large finite time, length, volume or similar scales.

One of the first surprises engineers encountered regarding solutions of governing equations on the theory of elasticity involved failures of structural components at stress
levels much smaller than the obtained stresses and strains would indicate. This was especially pronounced with brittle materials, while ductile materials such as aluminum were more resistant to sudden failure. Nevertheless, in the 1950s there was an infamous story of a British-made de Havilland DH 106 Comet passenger jet having a catastrophic structural failure in mid-air.

This was actually due to the development of “brittle like” dynamic fatigue cracks. The process of developing a brittle crack occurs basically at the micromechanical level of micro-structural elements of material (crystals, fibers, even atoms and molecules).

By extrapolating the continuum formulation to almost zero length and volume scales, for:

$$\sigma = \lim_{\Delta a \to 0} \frac{f}{\Delta a}$$

where $\sigma$ is the axial stress, $f$ is the axial load and $\Delta a$ is the cross section area, the whole micro-structure of a given material is automatically eliminated together with all emergent phenomena and emergent properties originating from this microstructure. Two of these eliminated phenomena are brittle and fatigue crack.

That said, problems of brittle fracture and fatigue have been addressed in a semi-empirical fashion that makes it possible to use continuum-based stress analysis in a design process.

A similar situation involving structural failure occurred in the well known collapse of the Malpasset Dam in 1959. The failure there happened due to a discontinuity in the rock mass under the foundation of the dam. This catastrophic collapse triggered the development of a whole set of science on discontinuous rock masses.

However, with the advent of present day science, the field of problems that are difficult to describe using governing differential equations has grown exponentially in recent years. These include traditional research and engineering problems such as mining, mineral processing, pharmaceuticals, medicine delivery techniques, fluid flow problems, problems of astrophysics, and also problems of nano-science and nano-technology, social sciences, biological sciences, economics, marketing, etc.

### 1.2 The Paradigm Shift

With the discovery of differential calculus a complete paradigm shift in how scientific problems were approached occurred. Differential calculus became a powerful enabling
technology in the hands of scientists and engineers that enabled the formulations of the most challenging problems in terms of mathematical equations. The first beneficiary of this discovery was, of course, Newtonian Mechanics.

In the course of dealing with differential problems further insights into powerful mathematical tools were gained. In dealing with stress analysis problems, it was soon realized that at a single material point P, as shown in Figure 1.4, stress can be described as a distributed internal force per unit area of a particular internal surface. The problem is that one can put many internal surfaces through the same point. Thus the stress at point P depends on what surface is chosen; in general, the stress on surface $n_1$ is different from the stress on surface $n_2$.

To solve this stress puzzle, the work of Cauchy and others led to the concept of a tensor and thus, tensorial calculus was developed. During the 1960s, Truesdell and Gurtin generalized the concept of a tensor and redefined it as a linear mapping that maps one vector into another. Stress then becomes a mapping from the vector space of surfaces to the vector space of forces. In a sense, for a given surface a particular internal force is assigned and if the surface doubles in size, so does the force – thus linear mapping. One could in theory represent this mapping using a spreadsheet; but this mapping is more conveniently represented using vector bases and matrices that describe the mapping (tensor) in a given vector base. Tensors as physical quantities became a powerful concept in describing stresses, strains, gravity, etc.

Formulating an engineering or scientific problem in terms of differential equations is much easier than solving these equations. In fact solutions in a closed analytical form rarely exist and engineers and scientists are forced to use approximate solutions of the governing differential equations.

A real revolution in our ability to solve governing partial differential equations occurred with the arrival of affordable silicon-chip-based computers. One could argue that the development of affordable computing hardware together with the accompanying computer languages was a milestone as important as the discovery of differential calculus itself and in modern science the two go together; one enables the formulation of the problem, while the other enables solving of the actual equations.

The problem is that all of these are based on the continuum assumption as explained above; there is a whole diverse field of problems, especially in modern science, that do not subscribe to this assumption. The crack propagation problem is one of the simplest of these. Another problem that does not subscribe to the assumption is flow through a very small diameter tube or a nano-tube. The diameter of the nano-tube is comparable to

![Figure 1.4](image)

**Figure 1.4** Distributed internal force for different surfaces.
the size of individual atoms, as shown in Figure 1.5, thus any smoothing of the micro-
structure through the continuum assumption automatically eliminates the most interesting
physical phenomena occurring at this length scale.

One could argue that this should be expected for very small scale problems. However,
even cosmic scale problems have similar properties to these smaller scale problems; in
rarefied gases the mean free path of the molecules is comparable to the physical scale of
the problem, therefore requiring one to account for discontinua effects.

Other examples where one must account for discontinua effects are: granular flow, rock
slides, spontaneous stratification, spraying, milling, shot pinning, mixing and other similar
industrial engineering and scientific problems. Even problems such as fire evacuation and
crowd control have the same discrete aspects.

In all these cases the physical behavior originates from interaction between individual
entities such as atoms, molecules, grains, particles, members of a crowd, etc. What one
needs to describe is the structure of the problem (that is, the individual entities such as an
initial position for each person in the crowd), the behavior of each individual entity (each
person in the crowd which may have different psychological aspects) and the interaction
between the individual entities (for example, individual members of the crowd pushing
each other).

To analyze a problem formulated in the above way one would require a computer
in order to solve the problem in this lifetime. However, there are no continuum based
governing equations based on averaging properties such as

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

(1.8)

The flowchart of formulating a discontinua problem is shown in Figure 1.6. In essence,
one can say that there is another fundamental paradigm shift in how some scientific
problems are approached. This paradigm shift can be proven as important and as essential
for the future of science as differential calculus was for past science.

This paradigm shift can be described as a move towards describing physical systems
using “discrete populations”. A discrete population can be a space occupied by individual
atoms that interact with each other. Motion of these atoms may produce a crystal or a
droplet of liquid or a gas phase of matter, where pressure consists of interaction between
individual atoms. The duration of these interactions are measured in femtoseconds.

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**Figure 1.5** Schematic representation of a cross section of Argon gas flow through a nano-tube.
Assemble discrete populations (individual entities)

Define interaction laws

Perform a virtual experiment

Observe the emergent properties and derive conclusions

Figure 1.6 Flowchart for the formulation of a Mechanics of Discontinua problem.

In a similar way a discrete population can be a sports arena that is occupied by individual spectators. Interactions between these spectators in emergency evacuations may produce emergent properties such as panic and stampede or a bottleneck.

A discrete population can also be composed of individual terrestrial bodies that attract each other through gravity which then leads to particle accretion and/or granular temperature.

A discrete population can be composed of the individual components of a tall building. An emergent property may be the progressive collapse produced by individual components falling and hitting other components, thus causing a domino effect.

Further generalization of the discrete population concept could be applied to a population of market participants interacting with each other through trading. An emergent property would be the stock market crash or property bubble.

A discrete population can be a biological ecosystem with interaction between individual players. An emergent property would be extinction or stock depletions.

In all the above presented cases, one arrives at the concept of discontinuum. The concept of continuum is based on smoothing out all the complexities of the micro-structure through an averaging process that “in the limit” produces instantaneous velocity or density at the point. This averaging process uses instantaneous or point limit averaged quantities and is naturally described using differential equations.

As opposed to the continuum concept, the discontinuum concept emphasizes the micro-structure of certain length scales. For example, it uses individual terrestrial objects rather than smoothing them through a density field, etc.

The discontinuum approach always concentrates at certain levels of discontinua such as the level of individual atoms, or the level of individual particles, or the level of individual humans, or the level of individual spectators, etc.

The applied science that deals with the formulation, simulation and solving of the problems of discontinua is called Mechanics of Discontinua. Mechanics of Discontinua is a relatively new discipline based on emphasizing the discontinuous nature of a given problem. An essential part of Mechanics of Discontinua is computer simulation leading to emergent properties.
1.3 Some Problems of Mechanics of Discontinua

1.3.1 Packing

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 engineering problems, one may arrive at a conclusion that engineering materials are well represented by a hypothetical continuum model. That this is not the case is easily demonstrated by the following problem:

A square base glass container is filled with particles of varying shapes and sizes as shown in Figure 1.7. The particulate is left to fall from a 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 particles come to a state of rest. The question to be answered is what is the total volume occupied by the particulate after they have come to their state of rest?

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

$$\rho = \frac{dm}{dV} \quad (1.9)$$

and the definition of mass $m$ given by

$$m = \int_V \rho dV \quad (1.10)$$

are not valid for the container problem.
For the problem shown in Figure 1.7, the total mass of the system is given by

\[ m = \sum_{i=1}^{N} m_i \]  

(1.11)

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 the individual particles. It is worth mentioning that the size of the container is not much larger than the size of the individual particles. The way the particles pack in the container and the mass of the particles in the container is a function of the size of the container, shape of individual particles, size of individual particles, deposition method, deposition sequence, etc.

For example, if the size of the particles is changed significantly, then the final density profile obtained inside the container is drastically affected, as shown in Figure 1.8.

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 the individual discrete elements (diameter of sphere in the problem described above) becomes small in comparison to the characteristic length of the problem being analyzed. In the container problem, the characteristic length of the problem is the length of the smallest edge of the box. Thus, 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 analyzed.

### 1.3.2 Fracture and Fragmentation

Fracture, and especially brittle fracture, was one of the early problems that required the continuum assumption to be mended in order to take into consideration the complex microstructural processes that produce fracture.

![Figure 1.8](image) Gravitational packs for different size distributions.
One of the amended theories was Griffith’s fracture energy release rate theory. Another approach is based on stress intensity factors. These are quite good in predicting single crack propagation mechanisms. However, when it comes to multiple cracks and/or complex fracture patterns these theories face numerous problems in describing the first principle physics that occur.

In many industrial engineering and scientific applications fracture, fracture patterns, and very often fragmentation play a key role in understanding these processes. In these cases, continuous based approaches are generally inadequate.

However, discontinuum based approaches have provided good predictions of even the most complex experimental fracture patterns such as those illustrated in Figures 1.9, 1.10 and 1.11. The results shown in these figures clearly demonstrate that the methods used

Figure 1.9  Symmetric triangular pulse of peak pressure 80 MPa and duration 1 ms.

Figure 1.10  Symmetric triangular pulse of peak pressure 200 MPa and duration 0.2 ms.
Figure 1.11 Symmetric triangular pulse of peak pressure 500 MPa and duration 0.05 ms.

Figure 1.12 Detonation gas driven fracture pattern.
in mechanics of discontinua are able to describe fracture and fragmentation processes accurately, including complex dynamic fracture patterns.

In Figure 1.9 a disk with a hole in its center is shown. The hole is subject to a symmetric triangular pulse of peak pressure of 80 MPa. Discontinua-based simulation produces a fracture problem that compares well with experimental results.

In addition, the discontinua-based simulation is able to capture the changes in the fracture pattern due to the changes in pressure pulse as shown in Figures 1.10 and 1.11. The fracture patterns shown in Figure 1.11 are quite different from the fracture patterns shown in Figure 1.9, even though the only differences between the two problems are the peak pressure and pulse duration.

In these cases the combined Finite-Discrete Element Method (FEM-DEM) was used to obtain the fracture patterns. The same method can be used to obtain complex fracture patterns driven by fluid flow through the cracks as shown in Figure 1.12, where a detonation gas driven fracture process is illustrated.

There are many important applications where these discontinua processes play a key role: petroleum engineering, geothermal energy, carbon sequestration, mining, powder ceramics, construction, excavation, demolition, rock crashing, etc.

1.3.3 Demolition and Structures in Distress, Progressive Collapse

With recent worldwide changes in design codes a decisive shift towards limit state analysis based on random sets has been made. Ultimately, in an ideal world one would take a given building or a structure and apply “what if” scenarios using computer based simulations and input parameters (loads, material properties, etc.) that are random variables. From the results of these simulations one would obtain the probability of a given structure failing or collapsing. These types of analysis could ultimately replace the traditional industrial safety factors.

Due to computer hardware constraints and other factors, these kinds of simulations are still within the research domain. Nevertheless, there are, even at present, needs to analyze the collapsing process of a structure. In Figure 1.13 a simulation of a demolition of a chimney stack is shown. Very often, these types of demolitions have to be executed quite carefully due to the spatial constraints for the falling debris.

Another case when a structure has to be analyzed in terms of the collapse process is the progressive collapse. This is best illustrated by the progressive collapse of tall buildings. The upper floors collapse and their kinetic energy progressively breaks the floors underneath them.

The collapse of the upper floors can be triggered by impact, explosion, fire or a similar catastrophic event. This event can be a relatively small energy process that in normal circumstances would only produce limited localized damage to the building. However, in a progressive collapse situation, this event acts as a trigger that initiates an energy release process that is orders of magnitude greater than the triggering event. This process is simply the transfer of the upper floor’s potential energy into kinetic energy. This kinetic energy acts as a sledge hammer that destroys the parts of the building that it hits. In turn, the newly broken parts start falling, accumulating extra kinetic energy and the process
Figure 1.13  Chimney stack demolition – collapse sequence and crashing against the ground.

Figure 1.14  Progressive collapse as an emergent property.

continues, Figure 1.14 captures this emergent property. This is, in essence, a complex process of failure, impact, fracture, fragmentation and eventual collapse. It is a Mechanics of Discontinua process wherein the progressive collapse is an emergent property.

There are situations where even local failure has important health and safety consequences. An example of this is the case where shattering glass windows with relatively high speed glass particles cause serious injuries, Figure 1.15.

1.3.4  Nanotechnology

In the early 1990s the advances made in manufacturing technologies, such as electro discharge machining, bulk silicon micro machining, surface silicon micro machining and
lithography galvanization, enabled the manufacturing of micron-size electro-mechanical devices with characteristic dimensions in the micron and sub-micron size range. Some examples of these kinds of devices are: accelerometers used to unfold airbag systems, the design of bioassay microfluidic networks to perform patterned drug delivery, etc.

A similar revolution is now underway with the unveiling of the next generation of medical procedures. These include robotic diagnostics, where literally the patient swallows a whole laboratory in a form of a robotic pill that travels through specific parts of the body, collecting and recording data.

There is ongoing research to basically produce micro and nano-scale robotic surgery based on a similar principle. The idea is relatively simple: a robotic surgical pill is delivered to the place where surgery is needed. The pill basically contains a whole surgery theater and through remote control it basically performs local surgery with precision and robustness that cannot be matched by the imprecise human hand. With this technique, it is envisioned that patient recovery would take hours or days instead of weeks or months; there are no scars and the scope for error is minimized. An example where this type of surgery could be applied is neurosurgical operations where any mistake would have serious consequences for the patient.

Another example for the need to go towards smaller and smaller length scales is photovoltaics where it is important to capture the whole light spectrum through manipulation of the nano-structure of the materials and maximization of the reactive surface area. Through manipulation of the nano-structure great efficiency gains can be achieved. Examples of these are carbon nano-tubes, manifold crystal structures such as graphene and similar.

Nature has been manipulating nano-structure of materials for millions of years. A good example of this is biological tissue. One could argue that it is the nano-structure of a specific tissue that does the whole work. It is at the molecular level that force generation in muscles occurs. It is at cell level that bone grows and heals and strengthens itself in response to the external load.

Figure 1.15 The combined finite-discrete element simulation of a glass window breakage under the effect of a planar pressure wave.
In the last couple of hundred years humans have manipulated materials in bulk quantities and most present day machinery exploits bulk properties of gases, liquids and solids – thus the engines and engine designers are not concerned about what is going on at the atomic level.

In contrast to these, all biological processes happen at the atomic level. For instance proteins are created by literally gluing one aminoacid at a time. If one cuts half of a leaf, the rest of the leaf continues with photosynthesis. This occurs because the photosynthesis “engine” is so small that a single leaf contains an extremely large number of them.

Human technologies are moving fast in this direction and nano-technology has a potential for completely changing industries and society. The best example is a computer chip that is made by an endless repetition of basically identical components.

The first experiments done on these micro and nano devices showed that when fluid flows through them, it does not behave in the same way as it does inside their macro-sized counterparts. In addition, the continuum based theories were not able to fully explain all the data that the experimental side was delivering at the time. Because of this, a strong development in the theoretical understanding of the physics of the fluid flow inside micro-devices has been seen in the last 15 to 20 years.

Due to the reduction of the dimensions (length scale changes), the surface effects start to have more influence on the behavior of the fluid, in addition, the inertial forces tend to have a small contribution, which means small values of Reynolds number. In the case of micro and nano-devices the flow is characterized by small values of Re. In macro systems small values of Re are generally linked to small values of fluid velocities. However, in the case of micro and nano-flows the occurrence of small Re is determined by the small values of the characteristic lengths and not necessarily by a small value of the mean fluid speed.

An important point to consider when dealing with micro and nano gas flows problems is the gas rarefaction phenomenon. Since the dimensions of the fluid passages become smaller, the rarefaction effects start to play a very important role in the fluid flow behavior. This is characterized by high values of the Knudsen number, given by

\[ Kn = \frac{\lambda}{l} \]  

where \( \lambda \) is the mean free path of the molecules and \( l \) is a characteristic length of the problem being studied. The mean free path of a gas is defined as the average distance traveled by the molecules in between two successive collisions with other molecules. The characteristic length, on the other hand, can be either a geometric length or a length over which macroscopic quantities have a large variation.

According to the Knudsen number the gas flow can be divided into four different regimes, as proposed by Schaaf and Chambre (1958):

- Free Molecular Flow for \( 10 < Kn \)
- Transitional Flow for \( 0.1 < Kn < 10 \)
- Slip Flow for \( 0.01 < Kn < 0.1 \)
- Continuum Flow for \( Kn < 0.01 \)  

In the continuum flow regime the characteristic length of the system is so large in comparison with the mean free path of the molecules that the fluid (gas) is treated as
a continuum medium. The discrete nature of the gas can be ignored and the classical Navier-Stokes equations are suitable for describing the behavior of the gas.

In the slip flow regime the characteristic length of the system is of the same order of magnitude of the mean free path of the gas molecules. The discontinuum nature of the gas begins to be more evident. However, the effects derived from this fact are mainly concentrated on the boundaries of the system. The bulk of the gas can still be described by the Navier-Stokes equations. By introducing some modifications to the way of handling the boundary conditions the gas-wall interactions (slip boundary conditions) can also be described with the Navier-Stokes equations.

In free molecular flow the distance between the molecules is so great that most of the interactions are between the gas molecules and the boundaries, that is, there are not so many interactions among the gas molecules. This regime is well described by the Boltzmann equation.

The most difficult regime to be addressed is the transitional flow regime. The gas in this case behaves as a granular material, and the flow resembles a granular flow.

### 1.3.5 Block Caving

Block caving is a miner-less method for extracting ores from the earth crust. The method consists in undercutting vast areas located under the ore-rich rocks, therefore creating the right conditions for ore extraction, as shown in Figure 1.16. Depending on the characteristics of the rocks containing the ore, once the undercutting is done, the rock located around the cleared area may cave naturally under the influence of gravity or it may need to be drilled and blasted. After the caving process starts, the resulting blocks of rock fall into a series of draw-bells that enable their collection. Once they are collected they can be transported outside of the mine.

Block caving has proved to be one of the cheapest ways of extracting ore from the earth. However, this is true only if the right conditions are ensured, that is, the ore handling facilities, the size of the draw-bells, the spacing between the draw-bells, etc.

The block caving process depends on a number of factors, such as: angles of subsidence, the shape of the undercut face, the orientation of the cave front, the failure zones,
fragmentation processes, etc. (Hustrulid and Bullock, 2001). In other words the optimum design for the block caving process needs careful analysis. Numerical computational tools are of great help. As fracture and fragmentation processes play an important role, methods of Mechanics of Discontinua are essential for robust simulations of block caving. One of these is the Combined Finite-Discrete Element Method. Typical results of discontinua-based simulations of block caving are shown in Figures 1.17 and 1.18, where rock blasting, fracture, fragmentation and granular flow are all integrated into the same simulation.

1.3.6 Mineral Processing

Milling is a process where particles of a given material are crushed until they are the desired size. The ball mill is one way of achieving these results. The ball mill consists of a big drum (usually between 5 and 10 m of diameter) with its axis set horizontally.

Mechanics of Discontinua based simulations have become a tool of choice in analyzing and designing mills and other mineral processing equipment, as shown in Figure 1.19.

1.3.7 Discrete Populations in General

A natural generalization of the discontinua concept are discrete populations. Discrete populations may comprise individual atoms or molecules. But they can also comprise individual sand or powder particles interacting with each other. In a similar way they can comprise large blocks of rock in coastal engineering projects that through interlocking defend a coastal stretch from erosion. Discrete populations can be bodies as large as individual planets interacting through gravity. Discrete populations can comprise sport
spectators interacting with each other through mechanical, vocal and psychological means in such a way that a stampede occurs.

In a similar way discrete populations can be market players interacting with each other through market transactions, thus producing market bubbles, market rallies, market crashes and similar emergent properties.

In all of these there are usually a large number of particles, bodies, agents, participants and so on. These interact with each other, thus producing emergent properties.

Atoms of Argon gas interact with each other and at very low temperatures form a liquid droplet. Both the liquid phase and the spherical shape of the droplet are emergent properties, Figure 1.20.
Unlike problems of Continuum Mechanics (which are described using differential equations), Mechanics of Discontinua problems are described by interactions between individual particles and behavior of these particles. As a result, obtaining solutions to Mechanics of Discontinua problems without using computers is nearly impossible. Thus, numerical simulations through virtual experiments are an essential part of Mechanics of Discontinua. In the rest of this book, Mechanics of Discontinua “state of the art” methods are described in detail.

**References**


**Further Reading**


