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Implémentation d'un logiciel de modélisation de la cinématique et du transfert thermique en milieu granulaire

Préparé par :
DERRICHE Kadda
CHERCHEF Kamel

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AKERMI Nacereddine	professeur "A" (Univ. Ibn Khaldoun)	Président
BENARIBA Aboubakeur	Maitre de Conférences "A" (Univ. Ibn Khaldoun)	Examinateur
MAKHFI Souad	Maitre de Conférences "B" (Univ. Ibn Khaldoun)	Examinateur
SAFA Ali	Maitre de Conférences "B" (Univ. Ibn Khaldoun)	Examinateur
ABOSHIGHIBA Hicham	Maitre de Conférences "B" (Univ. Ibn Khaldoun)	Encadrant

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Ibn Khaldoun University of Tiaret
Faculty of Applied Sciences
Department of Mechanical Engineering

GRADUATION THESIS

For the Award of the Master's Degree

Field : Sciences and Technology
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Topic

Implementation of a software for kinematics and thermal transfer modeling in granular media

Prepared by :
DERRICHE Kadda
CHERCHEF Kamel

Publicly defended on : 19 / 06 / 2024, in front of the jury composed of :

AKERMI Nacereddine	Senior lecturer "A" (Univ. Ibn Khaldoun)	President
BENARIBA Aboubakeur	Senior lecturer "A" (Univ. Ibn Khaldoun)	Examiner
MAKHFI Souad	Senior lecturer "B" (Univ. Ibn Khaldoun)	Examiner
SAFA Ali	Senior lecturer "B" (Univ. Ibn Khaldoun)	Examiner
ABOSHIGHIBA Hicham	Senior lecturer "B" (Univ. Ibn Khaldoun)	Supervisor

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Dedicated

to Our precious parents who have always sacrificed for our success

supported us, stood by us, entrusted us with their full confidence,

and always believed in us, in addition to providing us with a dignified education.

Their love has made us who we are today.

To our entire families - grandparents, aunts, uncles, and friends alike

whose encouragement and love have been a constant source of strength and inspiration.

Sommaire

List of Figures

List of Tables

Table of abbreviations acronyms

DEM	The Discrete Element Method
CFD	Computational Fluid Dynamics
FEM	Finite Element Method
DM	Discrete Methods
NSCD	Non Smooth Contact Dynamics
CD	Contact Dynamics
SCD	Smooth Contact Dynamics
GEM	Granular Element Method
MMQ	The Method of Quantum Mechanics
MA	The Atomic Method
MDM	Discrete Methods mesoscopic
SPH	Smoothed Particle Hydrodynamic

Nomenclature

Symbol	Unit	Signification
u	$[Pa.s]$	dynamic viscosity
ρ	$\left[\mathrm{kg/m^3}\right]$	Volumic mass
J	$\left[\ \mathrm{kg \cdot m^2}\right]$	The moment of inertia
v	$\left[\mathrm{m^2/s}\right]$	kinematic viscosity
D	$[m]$	Diameter
C_P	$[\mathrm{j/kg \cdot ^\circ C}]$	Specific heat
H	[m]	Smoothing length
v_i, v_j	$\left[\ \mathrm{m^3}\right]$	Particule volumes
λ	$[w/m \cdot ^\circ \mathrm{C}]$	Thermal conductivity
R	[m]	The radius of the particle
Q_{ij}	[j]	The amount of heat
T_i, T_j	$[^\circ \mathrm{C}]$	Particle temperatures
ț	$[s]$	the time
r_n	$[N]$	Normal force
$\dot{u}_n$	$[\ \mathrm{m/s}]$	Relative Velocity
$\dot{u}_t$	$[\ \mathrm{m/s}]$	tangential Velocity
m	[kg]	The reduced mass

G	Shear modulus
y	Poisson's ratio
a_i, a_j	The rays of the particles in contact
E_{ij}	The effective Young modules
k_n	Normal stiffness
E_i, E_j	Young modules of particles
F^{ext}	Vector of external efforts
R^a	Vector of internal efforts
u_n	The normal distance
c_n	The damping coefficient
k_t	Tangential stiffness
k_n	Normal stiffness
Bi	Number of Biot
x_i, x_j	The position of the particles
a	The vector of generalized accelerations
M	The generalized mass matrix of the system
n	The number of particles in the system
h	Plank's constant
Ψ	the wave function
ε	The depth of the potential well
g	The finite distance
u	The vector of generalized coordinates
$\dot{u}$	The vector of generalized velocities
m_p	The particle mass vector
r_p	The position vector of the particle
H_c	Contact conductance

GENERAL INTRODUCTION

GENERAL INTRODUCTION

Granular media is a type of independent grain collections that are widely used in powders, 3D printing metals, geomechanics, agriculture, and medicines. The modeling process is difficult because of the high number of particles and their interactions. Since the development of the discrete element method by Cundall as a solution to the modeling problem, this method has become the preferred choice for modeling this type of phenomenon. The aim of this work is to initiate the development of a general software based on this method to treat thermal conductivity coupled with the mechanical dynamics. The novelty of this study is in the introduction of the thermal aspect in a general way. The adopted approach is based on "Object Oriented Programming" technique which allows the software to be modular, easy to extend and to maintain. The initial version is created using the Python programming language due to the availability of a comprehensive set of libraries. This makes drafting idea easy and not too time consuming. The study is organized in three chapters. The first presents a literature review about the discrete element method (DEM), its development on granular media and the principle behind it. Then, chapter II is devoted to explain the mathematical formulation both for the granular mechanical dynamics as well as the heat transfer. The last chapter, that is to say the third, is devoted to the application of the DEM through 8 case studies, that get sophisticated gradually, starting from a simple free fall of a single particle and finishing with a complex granular mixing model in a cylindrical cavity. We finish this thesis with a general conclusion where we draw the most important results and propose some ideas for future work.

CHAPTER I

BIBLIOGRAPHIC SEARCH

Chapter I

BIBLIOGRAPHIC RESERCH

I.1 Introduction

The discrete element method initiated by P. Cundall and O. Strack [1] is one of most powerful tools. DEM can simulate particle motion and interaction between particles. It takes into account not only geometric and material effects obvious, such as the shape of the particles, the nonlinearity of the material, the viscosity, the friction, etc., but it also considers various effects. The physical field of the medium surrounding or even the chemical reaction [2].

Modelling of discrete granular materials has recently been largely accepted as a research tool to study the mechanical behaviour of materials granular [3].

The most fascinating and interesting problems in mechanics are generally the most difficult to solve. With today's IT capabilities, discrete problems can be solved even if a large number of components are The numerical methods used to solve such problems will be called discrete methods (DM).

In most cases, the problem must be infinitely subdivided into components infinitesimal, resulting in local governance equations (generally differential) involving infinite components. These problems are called "continuous" problems. In a continuous problem, it is assumed that the material studied is continuous and completely fills the space it occupies.

Since the computer's power is limited, continuous problems cannot be solved accurately only by mathematical techniques, and techniques mathematics are generally limited to very simple situations [4].

Considered as an alternative to continuous methods (differences, volumes and finite elements), the Discrete Element Method (DEM), also called Method Distinct Elements, appeared in the 70s and is nowadays booming. DEM offers the possibility to digitally model cinematic effects and dynamics induced by a large number of interacting particles.

Today, the DEM is undeniably considered as one of the methods most effective in modelling many applications in engineering, such as:

- granular flows
- the mechanics of powders
- the mechanics of rocks

More recently, DEM has been associated with other numerical methods such as methods of volumes and finite elements in coupled approaches to take advantage of the advantages of each method. The DEM new direction in the understanding of complex phenomena at very fine scales, unlike continuous methods, which are complicated especially in the presence of discontinuities.

Mainly, two types of discrete modelling appear in the literature, depending on whether the interactions between particles with regular laws are taken into account or no.

The first type of discrete modelling is based on the Non Smooth approach Contact Dynamics" (NSCD), using non-regular mechanics with counts interactions between particles without interpenetration. In this type of law, none flexibility at inter-particle contact is not allowed. Among the resolution methods for this type of law, we can cite the "Contact Dynamics" (CD) approach, developed by Jean and Moreau [5], who is able to deal with a large number of contacts with a implicit integration scheme.

The second type of modelling is based on the Smooth Contact approach Dynamics (SCD) which differs from the first (NSCD) by the possibility of a interpenetration between particles in contact. Among the discrete methods based on the SCD, we can cite the Discrete Element Method (DEM) proposed by Cundall [1], which assumes that the interaction between particles is governed by spring-type models and shock absorber. As part of the regular approaches, there is also the Granular Element Method (GEM) developed by Kishino [6]. Interactions at contacts

are modelled in the same way as in the DEM with the advantage of virtual damping to stabilize the system. This approach uses a iterative resolution.

I.1.1 Brief history of the DEM

Granular materials consist of moving particles independently of each other and interacting at the points of contact. This nature makes the mechanical behaviour of these types of materials very complex and, to this the definition of a law of conduct capable of representing all aspects of their behaviour remains an open problem.

For twenty years a numerical method has been developed for model the behaviour of this type of media. This method is called the Discrete Elements (DEM) treats a granular material as an assembly of interacting particles at the contacts that can be broken or formed to each step of the time. Most of the developments and applications of the Discrete elements are derived from the pioneering work of Cundall (1971,1974,1979), intended to two-dimensional modelling of fractured rock environments and of granular media formed of cylinders. We will also note the numerical method original developed by J.-J. Moreau (1979,1988) and M. Jean et al. (1993).

The DEM has made it possible in recent years to highlight and improve understand the local phenomena (geometric, kinematic, static) that are at the basis of the phenomena observed at the sample scale. In particular, it has enabled better understand the evolution of the internal structure of the environment during the solicitation, and could be used as an aid to the development of behavioural models for granular soils (Bathurst et al., 1988) [7].

History of the method

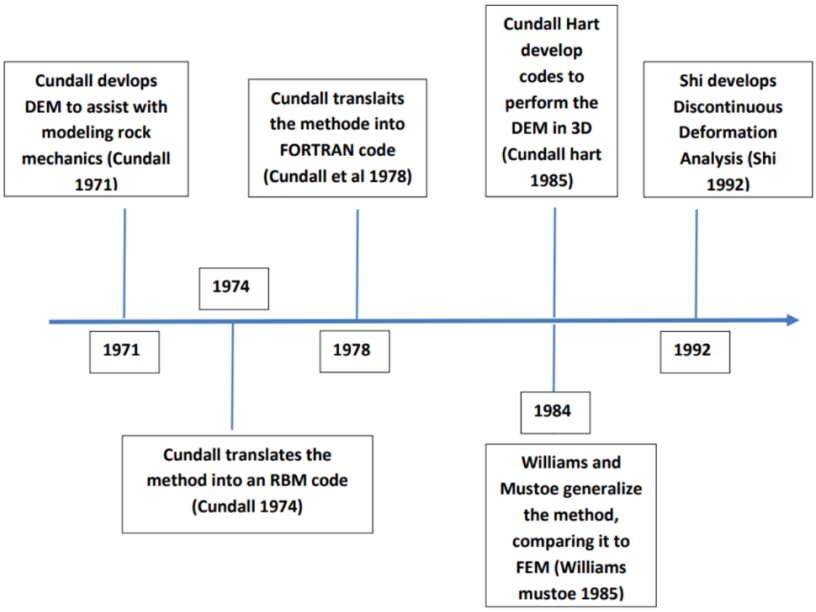


Figure I.1: History of the method

I.1.2 Differences between DEM and continuous methods

The discrete element method (DEM), originally used to study the granular materials, allows to address problems for which models based on the mechanics of continuous media are poorly adapted. However, several studies were conducted to model continuous materials with the DEM.

On the other hand, one of the difficulties lies in the choice of laws of interaction to find a satisfactory macroscopic behaviour. Among the methods The European Commission has recently developed microscopic, even nanoscopic scales. However, at this scale, the hypothesis of continuity of matter is no longer valid, and it is then necessary to take counts in the behaviour of a material, its local behaviour. Models of molecular dynamics allow to take into account the discontinuity of the matter at the nanoscale, but the shift from this scale to the scale of the A mechanical mechanism used to simulate the behaviour of a part or process is not possible with the current means of calculation. One of the solutions is to build a mesoscopic model that takes into account a large number of discontinuities, but on a scale to then simulate a volume compatible with a mechanical study. Models by discrete elements, historically developed for to model granular materials, are part of this perspective. In recent years, several studies have been carried

out to use the discrete elements for the simulation of continuous materials [8].

I.1.3 Classification of discrete methods

Depending on the scale of analysis, the most used DM in numerical simulation can be divided into three categories: the method of quantum mechanics (ab initio) (MMQ), the atomic method (MA) and mesoscopic MD (MDM) (Figure I-2)

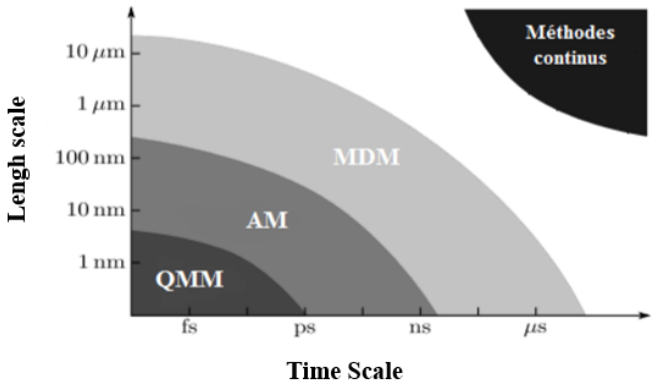


Figure I.2: Characteristic length and time scales for numerical methods

I.1.4 The principle of the DEM

The study of interacting grain collections is made possible by the DEM. It requires applying Newton's second rule, the fundamental law of dynamics, to compute the variation in the particles' angular momentum and quantity of motion, so describing the movement of the particles that make up the system. It is required to establish a strategy or algorithm in order to make distinct evolution elements of the numerical model (walls, particles, etc.) in time and space.

I.2 contact detection

The most costly DEM step is this one. It is dependent upon multiple elements, including geometry and particle count. Traditionally, all Ωj antagonists with $j >$ i are searched for neighbors for each particle Ωj . Once n, the number of grains in the sample, rises, one must conduct $\frac{n(n-1)}{2}$ checks, which quickly becomes expensive. Implementing an optimized contact detection technique is consequently important because the calculation time with such an approach grows as

so $O\left(n^2\right)$. Several methods exist in the literature to reduce the digital cost of contact detection. Among these techniques, there is the one proposed in [9], which consists in mapping the space study. Each particle located in a cell may be in contact with a particle neighbour located in the same or one of the 8 adjacent cells (Figure I.3- (a)). Another technique, called "halo" (Figure I.3- (b)), is to maintain for each particle the list of its nearest neighbors. Each particle is surrounded by a halo circular or square, of which it is the center, where only the particles located in this halo are taken into account in the detection of contacts.

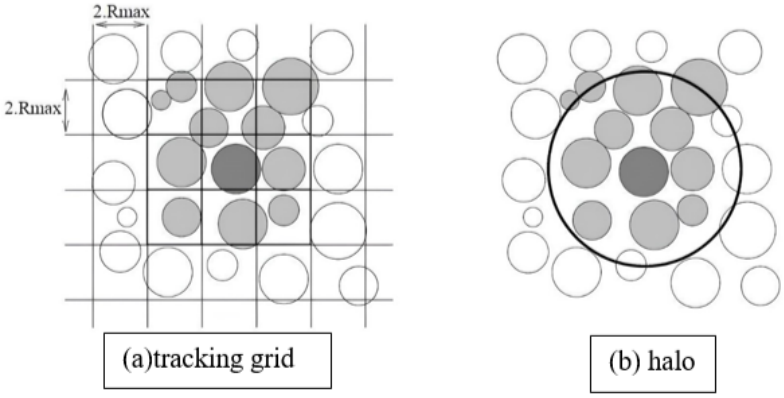


Figure I.3: Neighbour detection methods: (a) by locating in a fixed grid, (b) by the halo technique [10]

I.2.1 spatial discretization

The process of solving the system's dynamic equation is the foundation of numerical simulation for discrete media (multi-contact systems):

$$M\ddot{U} = F^{ext}(U,\dot{U},t) + R^{\alpha} \tag{I.1}$$

U: represents the vector of generalized coordinates (displacements and rotations);

$\dot{U}$: represents the generalized velocity vector (translation and angular);

$\ddot{U}$: represents the vector of generalized (translation and angular) accelerations;

M: represents the system's generalized mass matrix (diagonal matrix) with $M \in R^{n*n}$

n: refers to the number of particles in the system;

F^{ext}: Vector of external efforts;

R^{α}: Vector of internal efforts.

The solution is to use generalized coordinates and their first derivatives to calculate generalized accelerations when the system is subject to both internal and exterior forces. A resolution technique must be repeated step-by-step in the computation cycle, which is an algorithm.

I.2.2 Temporal discretization

The previous dynamic equation is discretized in time using a time integration scheme, such as the Newmark method. During each calculation cycle, we assess the contact links that are formed and broken between particles in the simulation. The interactions between particles are governed by a contact law, which is non-regular for "Non Smooth" cases and regular for Smooth cases. After calculating the resulting forces and moments on each particle, we solve the equation of motion to determine and update the new positions and velocities of the particles. Time integration schemes can be classified into two categories:

- Explicit
- Implicit

Explicit schemes are typically more cost-effective than implicit schemes, as the latter necessitate iterative calculations at every time step. However, it is worth noting that implicit patterns exhibit stability.

I.2.3 Verlet integration

Verlet integration, with its pronunciation derived from French, stands as a numerical method paramount in integrating Newton's equations of motion [11]. Widely employed in both molecular dynamics simulations and the realm of video games, this method offers superior stability when compared to the more simplistic Euler method. Beyond stability, Verlet integration exhibits other advantageous traits crucial for physical systems, including time-reversibility and the preservation of area.

While Euler integration may initially seem appealing for trajectory computations, it is plagued by numerous drawbacks, as elucidated in discussions surrounding Euler integration. The effectiveness of this technique hinges greatly on maintaining a uniform update rate or accurately

determining positions at a small temporal interval in the past.

Carl Stormer first applied Verlet integration to compute particle trajectories within magnetic fields, earning it the alternative designation of Stormer's method. Subsequently, French physicist Loup Verlet's popularization of the method in 1967 further cemented its significance, particularly in the domain of molecular dynamics.

I.2.4 Collision reactions

A penalty-based system is used to apply a specific force to a point upon contact as a method of dealing with collisions. However, it's challenging to determine the appropriate force to use. If it's too strong, objects may become unstable, and if it's too weak, they may pass through each other.

Another method is projection collision reactions, where the problematic point is moved the shortest distance possible to separate it from the other object. In this case, Verlet integration can handle the velocity resulting from the collision automatically. However, it may not always do so in a way that accurately reflects collision physics. Instead of automatically adjusting velocity, you would need to manually control the final velocities of the colliding objects by altering their recorded positions from the previous time step. The simplest approaches for determining new velocities are perfectly elastic collisions and inelastic collisions.

A more sophisticated approach involves using the coefficient of restitution, providing greater control over the collision outcome.

I.2.5 Calculation of the inter-articular force

The behavior of a granular medium under mechanical stress is significantly influenced by the contact network established among its particles. Therefore, selecting an appropriate interaction law is a crucial aspect of simulating the system using the DEM method. Various interaction laws can be utilized, with the most basic being the elastic contact law. This law governs the contact stress through two elastic parameters - normal kn and tangential kn stiffness, both of which are determined by the mechanical properties such as Young's modulus and Poisson's ratio.

I.2.6 Normal contact force

In the case of explicit modeling, the contact between two particles is established whether there is interpenetration, such as the normal distance $a > \beta$ with β ($\beta < 0$) a parameter close to zero which allows to control the approximation of the particle centers in contact: The normal force r_n is written according to the normal stiffness k_n and the normal distance one to through the following relationship:

$$R_n = K_n U_n \tag{I.2}$$

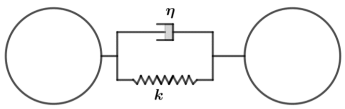


Figure I.4: Kelvin-Voigt contact model: spring k, damper !

I.2.7 Normal damping force

When two particles interact, energy is dissipated by friction as one particle slides toward the other. This dissipation is still not enough to reach steady state in a reasonable number of steps. Therefore, the inelastic quantity is taken into account in the contact model, this quantity is proportional to the viscous damping parameter C_n and is the derivative of the normal displacement $\dot{U}$.

The coefficient of depreciation C_n The European Commission has made it possible to stabilize the digital integration scheme. Viscous force is defined as:

$$r_n^v = -C_n \dot{U}_n \tag{I.3}$$

This force acts in opposition to relative displacement and is directly proportional to the relative speed, denoted as $\dot{U}$. When a viscous force is introduced, it can result in an adhesive state if

the repulsive force is significantly lower than the viscous force. To mitigate adhesion, one can reduce the calculated negative force to zero by accounting for the influence of the viscous force.

I.2.8 Tangential contact force

Calculating the tangential force r_t is calculated incrementally from The first contact detection is achieved by summing force increments Δr_t :

$$\Delta r_t = -K_t \Delta U_t \tag{I.4}$$

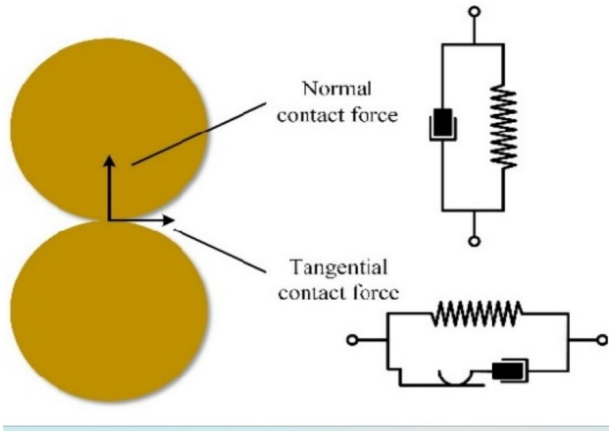


Figure I.5: Hertz–Mindlin no-slip model.[12]

The reaction that is tangential Δr_t^i The tangential reaction is taken into account at step i Δr_t^{i-1}. so at the previous time step i-1 It is given by the following relationship:

$$\Delta r_t^i = \Delta r_t^{i-1,act} + \Delta r_t \tag{I.5}$$

Where $\Delta r_t^{i-1,act}$ It goes beyond the actualization of the tangential reaction $\Delta r_t^{i-1,act}$. so which takes in counts the contact movement. The calculation for this amount involves both steps and takes counts the change in normal direction.

I.2.9 Tangential damping force

The presence of an inelastic (viscous) term is consistent with normal contact. introduced in the tangential interaction model. This is proportional to the coefficient amortizing C_t and depends

on the tangential speed $\dot{U}_t$. This force opposes the tangential displacement that is relative. The term inelastic is defined by viscous force following:

$$r_t^v = -C_t \dot{U}_t \tag{I.6}$$

I.2.10 Importance of Time Steps

The selection of the time step Δt is crucial in DEM. models. It must be selected small enough for two primary objectives: avoid excessive overlaps that could lead to excessively strong forces and minimize disruption effects waves, namely Rayleigh waves. A normal time interval for DEM is between 10 and 100, or 1e-4 and 1e-6 s. times smaller than what is often observed in computer CFD stands for fluid dynamics.

Rayleigh surface waves

Particle movement in granular flow is influenced by disturbances propagating from distant particles as well as interactions with nearby particles. Disturbance waves from each particle are stopped from spreading farther than their nearby neighbors by selecting a small enough time step in DEM. The Rayleigh surface wave propagation speed is used to approximate the suitable time step (Rayleigh time step). In order to guarantee realistic force transmission rates and avoid numerical instability, a fraction of this time step is typically taken.

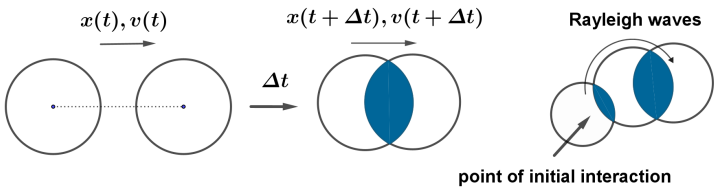


Figure I.6: Importance of Time Steps(Rayleigh surface waves)

I.3 General information about granular media :

Granular material is an aggregate of discrete solid particles dispersed in an interstitial fluid. Granular flows have many industrial applications including the transport of coal, ore, plastics, grains, mineral concentrates, sand, powders, foodstuffs or pharmaceuticals. Interactive particle collisions leading to random particle motions are the dominant mechanism influencing the flow behaviour. Because of the analogy between the random motion of particles in a granular flow and the motion of molecules in a gas, the theory of dense gas kinetics [13] is used. A collection of macroscopic solid particles, typically larger than $100\mu m$, is generally referred to as a granular medium [14].

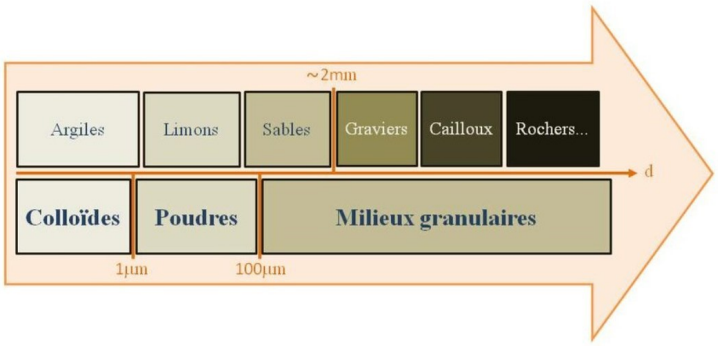


Figure I.7: Physical classification of media divided by particle diameter: collo ıdescollo ıdes, powders and granular media (Andreotti et al., 2011), (Pouliquen, 2001)[15]

I.3.1 Description of a granular mixture

The term ”granular mixture” refers to a medium composed of a finite number of families of particles of different diameters. The granular medium can be a wide range of very different materials: food products, chemicals, construction materials (concrete, soil, etc.), etc. Depending on the field of study, the relevant parameters of the granular medium are different: the presence or absence of water, the geometry of the particles, the granularity of the medium, the properties (such as friction) of the grains, the ordered or random nature of the medium, etc. Whatever the field of study, a granular medium is characterised by:

- Its porosity (or its complement, compactness), which corresponds to the percentage of void volume contained in the medium;

- The coordination numbers, which correspond to the average number of contacts per particle over the whole medium. For granular mixtures, an average coordination number is also determined for each family of granules, in which case they are called partial coordination numbers;

- The contact distribution of different types of contacts for granular mixtures only: a medium composed of different particle families presents different types of contacts: contacts between particles of the same family or between particles of two different families [16].

I.4 The Role of DEM in Simulation

Discrete element method (DEM) is a computational modeling framework used to simulate the behavior of granular and discontinuous bulk materials. Simulating bulk material is challenging because of the complex ways that the different discrete elements or particles interact with one another and with their surroundings. Bulk material does not exist in isolation: it is often interacts with a solid structure and is embedded in a surrounding fluid. In that sense DEM is an extension of traditional computational fluid dynamics (CFD) and finite element analysis (FEM). Granular flows are known to exhibit solid-like and fluid-like behaviors, or combination of both. To help accurately and efficiently simulate these bulk motions and their interactions with fluids and structures, python is introducing a brand-new product: python.

I.4.1 The different solution that used DEM

Various software packages are available for utilizing the Discrete Element Method (DEM) in simulations across different industries and research domains. Some examples include:

1. EDEM: EDEM is a leading DEM software used for simulating and analyzing the behavior of granular materials in industries such as mining, construction, pharmaceuticals, and food processing.

2. Rocky DEM: Rocky DEM offers high-performance DEM simulations for bulk material

handling, processing, and transportation industries. It specializes in particle dynamics and granular flow analysis.

3. LIGGGHTS: LIGGGHTS is an open-source DEM software tailored for simulating discrete particle systems, particularly in areas like granular flow, powder technology, and particulate processes.

4. YADE (Yet Another Dynamic Engine): YADE is an open-source DEM software developed for simulating complex particle interactions and granular materials behavior in various engineering and scientific applications.

Advantages:

1. Simulation Capabilities: DEM software enables the simulation of complex particle interactions and granular material behavior, providing valuable insights into real-world phenomena.

2. Engineering Applications: These software packages are widely used in various industries, including mining, pharmaceuticals, construction, and food processing, to optimize processes, improve product design, and enhance safety.

3. Customization: Many DEM software offer customization options, allowing users to tailor simulations to their specific needs and study a wide range of materials and conditions.

4. Visualization: Advanced visualization tools in DEM software help users interpret simulation results effectively, facilitating better understanding and decision-making.

5. Research and Development: DEM software serves as a crucial tool for researchers and developers to explore new materials, technologies, and processes, driving innovation and advancement in numerous fields.

Disadvantages:

1. Complexity: Using DEM software often requires a steep learning curve, particularly for users new to simulation techniques or programming/scripting languages.

2. Cost: Commercial DEM software packages can be expensive, especially for large-scale simulations or enterprise-level licenses, potentially limiting access for smaller organizations or academic institutions.

3. Resource Intensive: Running DEM simulations may require significant computational resources, including high-performance computing clusters or powerful workstations, leading to increased costs and longer simulation times.

4. Support and Documentation: Some DEM software packages may have limited documentation or technical support options, making it challenging for users to troubleshoot issues or learn new features.

5. Modeling Limitations: While DEM software offers powerful simulation capabilities, certain material behaviors or complex systems may be challenging to model accurately, requiring careful validation and calibration of simulation parameters.

6. Non-Thermal: It's important to note that DEM software typically focuses on the mechanical behavior of materials and does not inherently include thermal effects, requiring additional coupling with thermal simulation software for comprehensive analysis of thermomechanical systems.

I.4.2 Motivation for python as choice

Motivation for python as choice python is the fastest, most realistic DEM simulation product on the market. From candy to vacuum cleaners, nearly 70% of industrial products experience bulk granular material flows, where different-sized particles with complex shapes interact, potentially impacting a product's efficiency or structural integrity. To accurately and efficiently overcome this difficult design challenge, engineers require a DEM solution like python , with industry leading features, including:

- Complex particle shapes including flexible fibers and shells
- Accurate particle physics including breakage
- Integrated multibody dynamics

- Unique customization and automation APIs (Application Programming Interfaces)
- Python is free
- simple to use
- and offers a large library of tools and resources
- It is also available on multiple platforms
- users can leverage artificial intelligence (AI) capabilities within Python for enhanced simulations and analyses.

I.4.3 How the DEM Process Works with python

python is method that solves Newton's Second Law of Motion for each element/particle. The most important consideration for ensuring a high-fidelity simulation is to account for all the relevant forces acting on each particle. If the particles are still in range, the simulation will continue to cycle through this process. The heart of DEM implementation is accurate computation of the forces acting on every particle in the simulation. This requires a robust and accurate contact detection algorithm. Contact detection and the ability to handle shaped particles accurately is a critical differentiator between DEM codes. Standard DEM codes use a glued sphere approach. python uses polyhedral shapes, which have many advantages, including:

- Accurate shape representation including sharp corners and edges
- Actual particle shapes that give accurate particle-particle interactions
- Breakage modeling support

I.5 Exterior works

I.5.1 Correlation between hardness and abrasive wear of grinding balls:

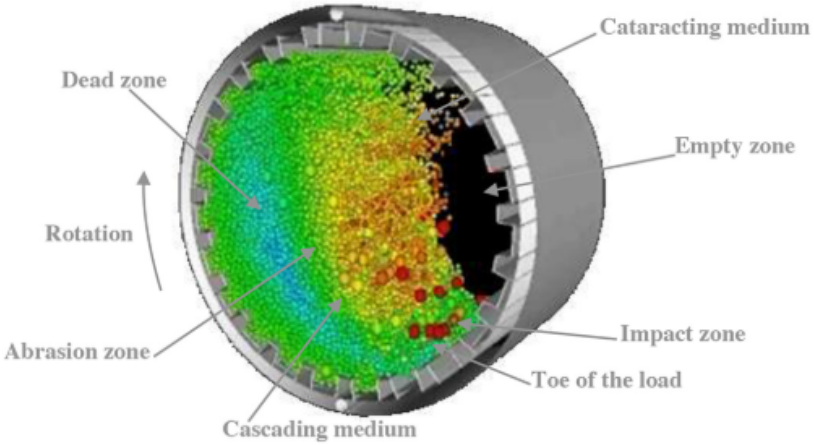


Figure I.8: Zones inside balls mill (dead zone, balls speed = zero)[17]

The grinding ball, manufactured by Algerian Foundries (ALFET – Tiaret), is essential for the cement industry to finely grind rock for cement production. This product is prone to significant wear, which manifests in two primary forms: abrasion and impact wear, each affecting its lifespan differently. Abrasion wear results from friction between surfaces such as rock, crusher shields, and the balls themselves, leading to mechanical disintegration and metal removal from these surfaces. Impact wear occurs when balls strike these surfaces from various angles, causing them to disintegrate upon impact. Generally, wear resistance increases with hardness; harder materials are less prone to seizing in the presence of abrasive particles and resist penetration into their surface layers. In this study, wear is quantified by measuring the mass loss of heat-treated balls. The research establishes a correlation between ball hardness and abrasive wear

Keywords: abrasion wear / impact wear / mechanical disintegration / correlation / hardness / mass loss / grinding balls / austenitizing temperature / quenching severity / tempering temperature

I.5.2 Improving Grinding Ball Lifespan And Efficiency Through Hardenability Modelling And Optimization:

Grinding balls, spherical or cylindrical components utilized in grinding and milling operations, are crafted from high chromium white cast iron (HCWCI) for various industrial processes. These balls play a pivotal role in reducing particle size to achieve finer products. The efficiency of grinding processes heavily depends on their composition, size, and hardness, prompting ongoing research to enhance their performance and durability against severe wear and impact conditions that shorten their lifespan. This study involved heat treating balls with diameters of 50 mm and 70 mm at temperatures of 950°C and 1050°C, followed by quenching using oil and compressed air. Using experimental Rockwell hardness (HRC) results, the study aimed to develop a mathematical model correlating the response (hardenability) with key factors: austenitization temperature, quenching medium, and ball diameter, along with their interactions. Analysis of variance (ANOVA) was employed to determine significant parameters, and the optimization of response was conducted using the best sub-models method and the desirability function in the latter part of the study. The findings indicate that austenitization temperature and ball size exert a more significant influence on ball hardenability compared to the cooling rate (quenching medium), thereby minimizing the hardness differential between the ball's surface and core to negligible levels. This research contributes valuable insights into optimizing the heat treatment process of grinding balls to enhance their performance under demanding operational conditions [17].

CHAPTER II

MATHEMATICAL FORMULATION

Chapter II

MATHEMATICAL FORMULATION

II.1 Introduction

To have an approximate solution, the numerical modelling of an environment heterogeneous can be achieved by various numerical approaches. This chapter presents the principles of the discrete element method, which is more suitable for discontinuity, but can also treat continuous media such as structures with heterogeneities.

II.2 Heat Transfer

Heat transfer is the movement of energy between materials due to a difference in temperature. There are three types of heat transfer: conduction, convection and radiation. Conduction is the mode of heat transfer in which energy exchange occurs in solids or liquids at rest (i.e. without convective motion resulting from the movement of the macroscopic part of the medium) from the high temperature region to the low temperature region. Molecules in liquids and gases have freedom of movement and when they move from a hot to a cold region they carry energy with them. The transfer of heat from one region to another due to such macroscopic motion in a liquid or gas, in addition to the transfer of energy by conduction in the fluid, is called convective heat transfer. All bodies emit heat radiation at all temperatures. This is the only type of heat transfer that does not require a material medium. Temperature is a scalar quantity which describes the specific internal energy of a substance. The temperature distribution in a body is determined as

a function of position and time, and then the heat flow in the body is calculated from the heat flow and temperature gradient laws [18].

II.2.1 Heat transfer in particulate systems

Conductive heat transfer is represented by the Fourier relation. These are the heat flows within each particle and these heat flows will occur once a temperature gradient is established in the solid. The second type of heat transfer in our model is physical contact between particles. This phenomenon can be quantified by the contact conductance between particles, which is strongly influenced by the properties of the contact element and the thermophysical properties. The heat flux transferred between two particles i and j is modelled by the contact conductance:

$$Q_{ij} = H_c \times (T_j - T_i) \tag{II.1}$$

Where Q_{ij} is the amount of heat from particle i received by particlej, H_c is the contact conductance,T_i and T_j are the temperatures of particles i and j respectively. Data on contact conductance are scarce and strongly related to the nature and thermophysical properties of the elements in contact. The evolution of the temperature of particle i, considering that it is in contact with N neighbouring particles, is given by the following expression (whereρ $.C_p.V$ is the heat capacity of the particle).

$$\rho.C_p \cdot V \cdot \frac{dT}{dT} = \sum_{j=1}^{N} H_c \left(T_j - T_i\right) \tag{II.2}$$

II.3 Heat conduction

Conduction is the transfer of energy from the most energetic particles of a substance to neighbouring, less energetic particles as a result of interactions between the particles. Conduction can occur in solids, liquids or gases. In gases and liquids, conduction is due to collisions and diffusion of molecules during their random motion. In solids, it is due to a combination of vibrations of molecules in a lattice and the transport of energy by electrons. The rate of heat conduction through a medium depends on the geometry, thickness and material of the medium, as well as the temperature difference across the medium [19].

II.3.1 Fourier's law

For heat conduction, the rate equation is known as Fourier's law, which for a homogeneous, isotropic solid (i.e. a material in which the thermal conductivity is independent of direction) is expressed as:

$$\vec{q}(\vec{r},t) = -\lambda \vec{\nabla} T(\vec{r},t) \tag{II.3}$$

where $\vec{\nabla} T(\overrightarrow{r,t})$ is the temperature gradient vector normal to the surface (C°/m), the heat flux vector heat flux vector $\overrightarrow{q}(\overrightarrow{r},t)$ is the heat flux per unit time and unit area of the isothermal surface in the direction of decreasing temperature (W/m^2), and λ is the thermal conductivity of the material, which is a positive scalar quantity $(W/m^2.C^\circ)$[19].

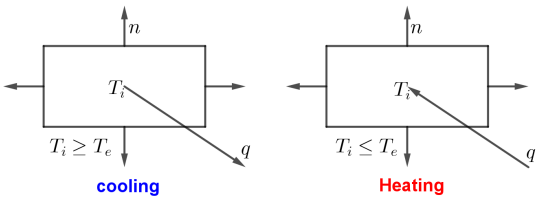


Figure II.1: The heat flow is in the hot/cold direction.

II.3.2 Thermal conductivity

Thermal conductivity λ is the quotient of heat flux density and temperature gradient. it corresponds to the amount of energy passing between two surfaces of one unit area separated by one unit length and is expressed in $(W/m.C^\circ)$ [20].

II.4 The Biot number

The Biot number is a number that expresses the balance between the resistance to heat transfer between particles and that through the particle itself. If the resistance between the particles is too large compared to the resistance inside the particle (which is expressed by a very small Biot number), the temperature field inside the particle will quickly become uniform. Equation (I.3)

assumes that the temperature of each particle is uniform. It is therefore necessary to check that the resistance of the flux transmitted in each particle is significantly lower than the resistance of the two particles in contact:

$$B_i = \frac{H_c}{\lambda \cdot \pi \cdot R} \ll 1 \tag{II.4}$$

Where B_i is the Biot number, λ and R are the thermal conductivity and radius of the particle respectively [21].

II.5 The numerical model by the discrete element method

The particles crash on their neighbors and deform under the influence of an external load or the weight of the particles themselves (in the case of a vertical stack). Le broyage est effectué sur une surface plane de géométrie circulaire. Cette situation est simplifiée en une interpénétration sans déformation dans le cadre de la méthode des éléments discrets. The amount of heat that is passed through the contact area under influence of a unit of temperature difference in a period of one unit of time (1s) is known as the conductance between the two particles. When two spherical particles i and j of the same nature (same material) come into contact, it is given by:

$$H_{ij} = 2kr_{c_{ij}} \tag{II.5}$$

With:

H_{ij}: Conductance between particles i and j

K: Thermal conductivity

$r_{c_{ij}}$: The radius of the (circular) contact zone between particles i and j. The amount of heat transferred from particle j to particle i through the contact area in one second is:

$$\dot{Q}_{ij} = H_{ij}\left(T_j - T_i\right) \tag{II.6}$$

With:

T_i: The particle temperature i

T_j: The particle temperature j. If the particle comes into touch with N other particles, the

quantity of total heat per unit time $\dot{Q}_{ij}$ will be as follows since the amount of heat is a scalar magnitude that can be either positive or negative.

$$\dot{Q}_i^T = \sum_{j=1}^{N_p} \dot{Q}_{ij} = \sum_{j=1}^{Np} H_{ij}\left(T_j - T_i\right) \tag{II.7}$$

And the relationship with temperature will be given by the following differential equation:

$$\frac{dT_i}{dT} = \frac{1}{c_p m_p}\dot{Q}_i^T = \frac{1}{c_p m_p}\sum_{j=1}^{N_p} \dot{Q}_{ij} \tag{II.8}$$

C_p: The specific heat of the particle;

m_p : The mass of the particle ;

$\frac{dT_i}{dT}$: The temporal derivative of temperature. The temporal derivative can be approximated by finite difference as follows:

$$\frac{dT_i}{dt} \approx \frac{T_i^{K+1} + T_i^K}{\Delta t} \tag{II.9}$$

And the differential equation can be approximated as:

$$\frac{T_i^{K+1} + T_i^K}{\Delta t} \approx \frac{1}{c_p m_p}\sum_{j=1}^{N_p} \dot{Q}_{ij}^K \tag{II.10}$$

So we can explicitly calculate the temperature of the particle i at the new moment T_i^{K+1} depending on the temperature values of the same particle and its immediate neighbors preceding T_i^K:

$$T_i^{K+1} \approx T_i^K + \frac{\Delta t}{c_p m_p}\sum_{j=1}^{N_p} \dot{Q}_{ij}^K \tag{II.11}$$

II.6 Verlet integration

II.6.1 Basic Verlet

Newton's equation of motion for conservative physical systems is

$$M\ddot{x}(t) = F(x(t)) = -\nabla V(x(t)) \tag{II.12}$$

or individually

$$m_k \ddot{\vec{x}}_k(\mathrm{t}) = F_k(x(t)) = -\nabla_{\vec{x}_k} V(x(t)) \tag{II.13}$$

Where

- t is the time,
- $x(t) = (\overrightarrow{x_1}(t), ..., \overrightarrow{x_N}(t))$ is the ensemble of the position vector of N objects,
- V is the scalar potential function,
- F is the negative gradient of the potential giving the ensemble of forces on the particles,
- M the mass matrix, typically diagonal with blocks with mass m_k for every particle. This setting allows to express problems in molecular dynamics and N-body planetary or stellar simulations, among others. After a transformation to bring the mass to the right side and forgetting the structure of multiple particles, the equation may be simplified to

$$\ddot{\vec{x}}(t) = A(\vec{x}(t)) \tag{II.14}$$

with some suitable vector valued function A representing the position dependent acceleration. Typically, an initial position $\overrightarrow{x}(t) = \overrightarrow{x_0}$ and an initial velocity $\overrightarrow{v}(0) = \dot{\overrightarrow{x_0}} = \overrightarrow{v_0}$ are also given To discretize and numerically solve this initial value problem, a time step $\Delta t > 0$ is chosen and the sampling point sequence $t_n = n\Delta t$ considered. The task is to construct a sequence of points $\overrightarrow{x_n}(t)$ that closely follow the points $\overrightarrow{x}(t_n)$ on the trajectory of the exact solution. Where Euler's Method uses the forward difference approximation to the first derivative in differential equations of order one, Verlet Integration can be seen as using the central difference approximation to the second derivative:

$$\frac{\Delta^2 \vec{x}_n}{\Delta t^2} = \frac{\frac{\vec{x}_{n+1} - \vec{x}_n}{\Delta t} - \frac{\vec{x}_n - \vec{x}_{n-1}}{\Delta t}}{\Delta t} = \frac{\vec{x}_{n+1} - 2\vec{x}_n - \vec{x}_{n-1}}{\Delta t^2} = \vec{a}_n = A(\vec{x}_n) \tag{II.15}$$

The Verlet algorithm [23] uses this equation to obtain the next position vector from the previous two as

$$\vec{x}_{n+1} = 2\vec{x}_n - \vec{x}_{n-1} + \vec{a}_n \Delta t^2, \vec{a}_n = A(\vec{x}_n) \tag{II.16}$$

without using the velocity. The time symmetry inherent in the method reduces the level of errors introduced into the integration by calculating the position at the next time step. The error is quantified by inserting the exact values ($\overrightarrow{x}(t_{n-1}), \overrightarrow{x}(t_n), \overrightarrow{x}(t_{n+k})$) into the iteration and computing the Taylor expansions at time $t = t_n$ of the position vector $\overrightarrow{x}(t \pm \Delta t)$ in different time directions.

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{\vec{a}(t)\Delta t^2}{2} + \frac{\vec{b}(t)\Delta t^3}{6} + O\left(\Delta t^4\right) \tag{II.17}$$

$$\vec{x}(t-\Delta t) = \vec{x}(t) - \vec{v}(t)\Delta t + \frac{\vec{a}(t)\Delta t^2}{2} - \frac{\vec{b}(t)\Delta t^3}{6} + O\left(\Delta t^4\right) \tag{II.18}$$

where is $\overrightarrow{x}$ the position, $\overrightarrow{v} = \dot{\overrightarrow{x}}$ the velocity, $\overrightarrow{a} = \ddot{\overrightarrow{x}}$) the acceleration $\overrightarrow{b}$ and the jerk (third derivative of the position with respect to the time)t. Adding these two expansions gives

$$\vec{x}(t+\Delta t) = 2\vec{x}(t) - \vec{x}(t-\Delta t) + \vec{a}(t)\Delta t^2 + O\left(\Delta t^4\right) \tag{II.19}$$

We can see that the first and third-order terms from the Taylor expansion cancel out, thus making the Verlet integrator an order more accurate than integration by simple Taylor expansion alone. Caution should be applied to the fact that the acceleration here is computed from the exact solution, $\overrightarrow{a}(t) = A(\overrightarrow{x})$, whereas in the iteration it is computed at the central iteration point, $\overrightarrow{a_n} = A(\overrightarrow{x}_n)$. In computing the global error, that is the distance between exact solution and approximation sequence, those two terms do not cancel exactly. Note that at the start of the Verlet-iteration at step $n = 1$, time $t = t_1 = \Delta t$, computing $\overrightarrow{x_2}$, one already needs the position vector$\overrightarrow{x_2}$ at time $t = t_1$. At first sight this could give problems, because the initial conditions are known only at the initial time. However, from these the acceleration $\overrightarrow{a_0} = A(\overrightarrow{x}_0)$. is known, and a suitable approximation for the first time step position can be obtained using the Taylor polynomial of degree two:

$$\vec{x}_1 = \vec{x}_0 + \vec{v}_0\Delta t + \frac{1}{2}\vec{a}_0\Delta t^2 \approx \vec{x}(\Delta t) + O\left(\Delta t^3\right) \tag{II.20}$$

The error on the first time step calculation then is of order $O(\Delta t^3)$. This is not considered a problem because on a simulation of over a large amount of timesteps, the error on the first timestep is only a negligible small amount of the total error, which at time t_n is of the order ,

$\Theta(e^{IA_n}\Delta t^2)$ both for the distance of the position vectors $\overrightarrow{x_n}$ to $\overrightarrow{x}(t_n)$ as for the distance of the divided differences $\frac{\overrightarrow{x}_{n+1}-\overrightarrow{x}_n}{\Delta t}$ to $\frac{\overrightarrow{x}(t_{n+1})-\overrightarrow{x}(t_n)}{\Delta t}$. Moreover, to obtain this second order global error, the initial error needs to be of at least third order. The velocities are not explicitly given in the Basic Verlet equation, but often they are necessary for the calculation of certain physical quantities like the kinetic energy. This can create technical challenges in molecular dynamics simulations, because kinetic energy and instantaneous temperatures at time t cannot be calculated for a system until the positions are known at time $t+\Delta t$. This deficiency can either be dealt with using the Velocity Verlet algorithm, or estimating the velocity using the position terms and the mean value theorem:

$$\vec{v}(t) = \frac{\vec{x}(t+\Delta t) - \vec{x}(t-\Delta t)}{2\Delta t} + O\left(\Delta t^2\right) \tag{II.21}$$

Note that this velocity term is a step behind the position term, since this is for the velocity at time t, not $t+\Delta t$, meaning that $\overrightarrow{v}_n = \frac{\overrightarrow{x}_{n+1}-\overrightarrow{x}_{n-1}}{2\Delta t}$ is an order two approximation to $\overrightarrow{v}(t_n)$. With the same argument, but halving the time step $\overrightarrow{v}_{n+1/2} = \frac{\overrightarrow{x}_{n+1}-\overrightarrow{x}_n}{\Delta t}$, is an order two approximation to $\overrightarrow{v}(t_{n+1/2})$, with $t_{n+1/2} = t_n + \frac{1}{2}\Delta t$ One can shorten the interval to approximate the velocity at time at the cost of accuracy:

$$\vec{v}(t+\Delta t) = \frac{\vec{x}(t+\Delta t) - \vec{x}(t)}{\Delta t} + O(\Delta t) \tag{II.22}$$

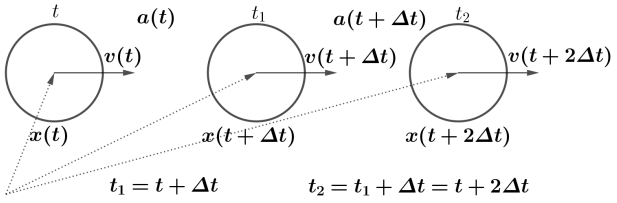


Figure II.2: Single element motion calculation in terms of acceleration, velocity and position in DEM

II.6.2 Velocity Verlet

A related, and more commonly used, algorithm is the Velocity Verlet algorithm [24], similar to the Leapfrog method, except that the velocity and position are calculated at the same value of the time variable (Leapfrog does not, as the name suggests). This uses a similar approach but explicitly incorporates velocity, solving the first-timestep problem in the Basic Verlet algorithm:

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2 \tag{II.23}$$

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{\vec{a}(t)+\vec{a}(t+\Delta t)}{2}\Delta t \tag{II.24}$$

It can be shown that the error on the Velocity Verlet is of the same order as the Basic Verlet. Note that the Velocity algorithm is not necessarily more memory consuming, because it's not necessary to keep track of the velocity at every timestep during the simulation. The standard implementation scheme of this algorithm is:

1. Calculate:
$$\vec{v}\left(t+\frac{1}{2}\Delta t\right) = \vec{v}(t) + \frac{1}{2}\vec{a}(t)\Delta t \tag{II.25}$$

2. Calculate:
$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}\left(t+\frac{1}{2}\Delta t\right)\Delta t \tag{II.26}$$

3. 3.Derive $\overrightarrow{a}(t+\Delta t)$ from the interaction potential using $\overrightarrow{x}(t+\Delta t)$

4. Calculate:
$$\vec{v}(t+\Delta t) = \vec{v}\left(t+\frac{1}{2}\Delta t\right) + \frac{1}{2}(\vec{a}(t+\Delta t)\Delta t) \tag{II.27}$$

Eliminating the half-step velocity, this algorithm may be shortened to

1. Calculate:
$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{1}{2}\vec{a}(t)\Delta t^2 \tag{II.28}$$

2. Derive $\overrightarrow{a}(t+\Delta t)$ from the interaction potential using $\overrightarrow{x}(t+\Delta t)$

3. Calculate:

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{1}{2}\left(\vec{a}(t) + \vec{a}(t+\Delta t)\right)\Delta t \tag{II.29}$$

Note, however, that this algorithm assumes that acceleration $\overrightarrow{a}(t+\Delta t)$ only depends on position $\overrightarrow{x}(t+\Delta t)$, and does not depend on velocity $\overrightarrow{v}(t+\Delta t)$. One might note that the long-term results of Velocity Verlet, and similarly of Leapfrog are one order better than the Semi-implicit Euler method. The algorithms are almost identical up to a shifted by half of a timestep in the velocity. This is easily proven by rotating the above loop to start at Step 3 and then noticing that the acceleration term in Step 1 could be eliminated by combining Steps 2 and 4. The only difference is that the midpoint velocity in Velocity Verlet is considered the final velocity in Semi-implicit Euler method. The global error of all Euler methods is of order one, whereas the global error of this method is, similar to the Midpoint method, of order two. Additionally, if the acceleration indeed results from the forces in a conservative mechanical or Hamiltonian system, the energy of the approximation essentially oscillates around the constant energy of the exactly solved system, with a global error bound again of order one for semi-explicit Euler and order two for Verlet-leapfrog. The same goes for all other conservered quantities of the system like linear or angular momentum, that are always preserved or nearly preserved in a symplectic integrator. [22]

Error terms

The local error in position of the Verlet integrator is $O(\Delta t^4)$ as described above, and the local error in velocity is $O(\Delta t^2)$ The global error in position, in contrast, is $O(\Delta t^2)$ and the global error in velocity is $O(\Delta t^2)$. These can be derived by noting the following:

$$\left(x\left(t_0+\Delta t\right)\right) = O\left(\Delta t^4\right) \tag{II.30}$$

And

$$x(t+2\Delta t) = 2x\left(t_0+\Delta t\right) = x\left(t_0\right) + \Delta t^2 x''\left(t_0+\Delta t\right) + O\left(\Delta t^4\right) \tag{II.31}$$

Therefore:

$$\text{error} \quad (x(t_0+\Delta t)) = 2\,\text{error}\,(x(t_0+\Delta t)) + O\left(\Delta t^4\right) = 3O\left(\Delta t^4\right) \tag{II.32}$$

Similarly:

$$\text{error} \quad (x(t_0+3\Delta t)) = 6O\left(\Delta t^4\right) \tag{II.33}$$

$$\text{error} \quad (x(t_0+4\Delta t)) = 10O\left(\Delta t^4\right) \tag{II.34}$$

$$\text{error} \quad (x(t_0+5\Delta t)) = 15O\left(\Delta t^4\right) \tag{II.35}$$

Which can be generalized to (it can be shown by induction, but it is given here without proof):

$$\text{error} \quad (x(t_0+3\Delta t)) = \frac{n(n+1)}{2} O\left(\Delta t^4\right) \tag{II.36}$$

If we consider the global error in position between $x(t)$ and $x(t+T)$, where $T = n\Delta t$, it is clear that:

$$\text{error} \quad (x(t_0+T)) = \left(\frac{T^2}{2\Delta t^2} + \frac{T}{2\Delta t}\right) O\left(\Delta t^4\right) \tag{II.37}$$

And therefore, the global (cumulative) error over a constant interval of time is given by:

$$\text{error} \quad (x(t_0+T)) = O\left(\Delta t^2\right) \tag{II.38}$$

Because the velocity is determined in a non-cumulative way from the positions in the Verlet integrator, the global error in velocity is also $O(\Delta t^2)$. In molecular dynamics simulations, the global error is typically far more important than the local error, and the Verlet integrator is therefore known as a second-order integrator.

II.7 Model for 2 particles:

II.7.1 Modelling of thermal conductivity by MED

An interpenetration without deformation is used to simulate particle interaction in the context of the discrete element method. The geometric parameters of the contact area (particle distance,

contact area and radius, etc.)

Area of Intersection:

The intersection area (CD in the figure below) is circular its radius (ED or EC) is determined by the following steps:

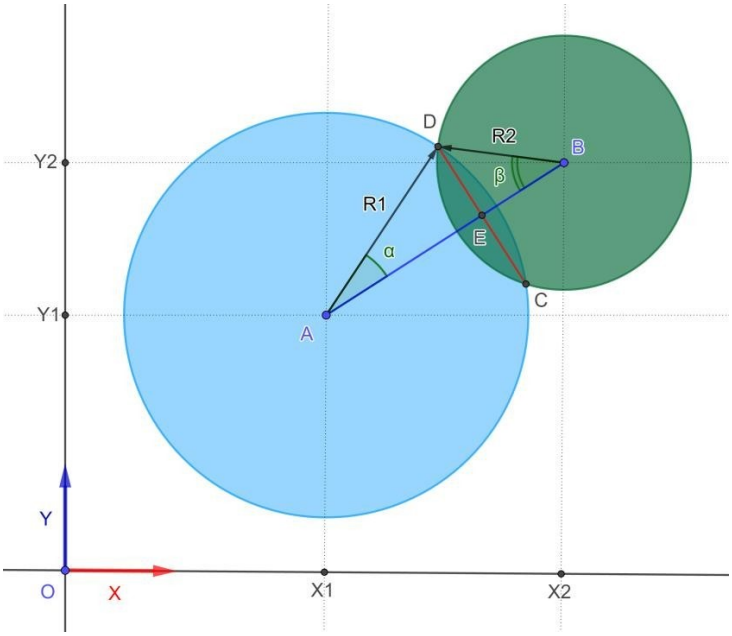


Figure II.3: Interpenetration between two spherical particles

The conductivity between the two particles is measured in terms of the amount of heat exchanged. transported through the contact area under the influence of a unit of difference Temperature in a unit of time (1s). The measurement of conductivity between two particles serves as a crucial parameter, quantified by the heat exchanged and transported through the contact area. This conductivity evaluation is conducted within the framework of a unit temperature difference over a specified unit of time, typically one second. The efficiency of heat transfer between particles is thus precisely assessed, offering valuable insights into the thermal dynamics of the system. This method provides a quantitative understanding of the thermal conductivity, allowing for the characterization of materials and the optimization of processes reliant on heat

exchange.

$$L = AB = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

$$\begin{cases} DE^2 = R_1^2 - AE^2 \\ DE^2 = R_2^2 - BE^2 \end{cases}$$

$$BE = L - AE$$

$$R_1^2 - AE^2 = R_2^2 - BE^2$$

$$R_1^2 - AE^2 = R_2^2 - (L - AE)^2$$

$$R_1^2 - AE^2 = R_2^2 - \left(L^2 - 2L \cdot AE + AE^2\right)$$

$$R_1^2 = R_2^2 - \left(L^2 - 2L \cdot AE\right)$$

$$R_1^2 = R_2^2 - L^2 + 2L \cdot AE$$

$$AE = \frac{R_1^2 - R_2^2 + L^2}{2L}$$

$$DE = \sqrt{R_1^2 - \left(\frac{R_1^2 - R_2^2 + L^2}{2L}\right)^2}$$

The area is therefore given by:

$$a = \pi r^2 = \pi DE^2 = \pi \left(R_1^2 - \left(\frac{R_1^2 - R_2^2 + L^2}{2L}\right)^2\right)$$

$$\text{Penet} = R_1 + R_2 - L$$

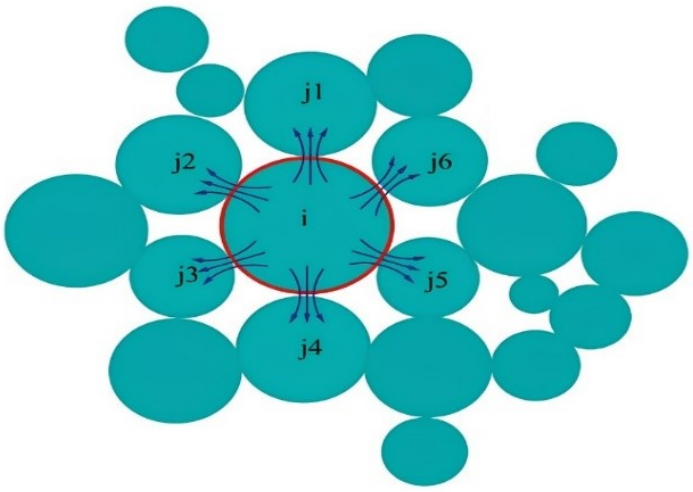


Figure II.4: Interpenetration between two particles[23]

II.8 Model for n particles:

The total amount of heat per unit of time, $\dot{Q}_I^T$, will be the algebraic sum of the quantities of heat exchanged by each of the neighboring particles because the amount of heat is a scalar magnitude, which can be positive or negative, if the i^{eme} particle is in contact with N_P particles.

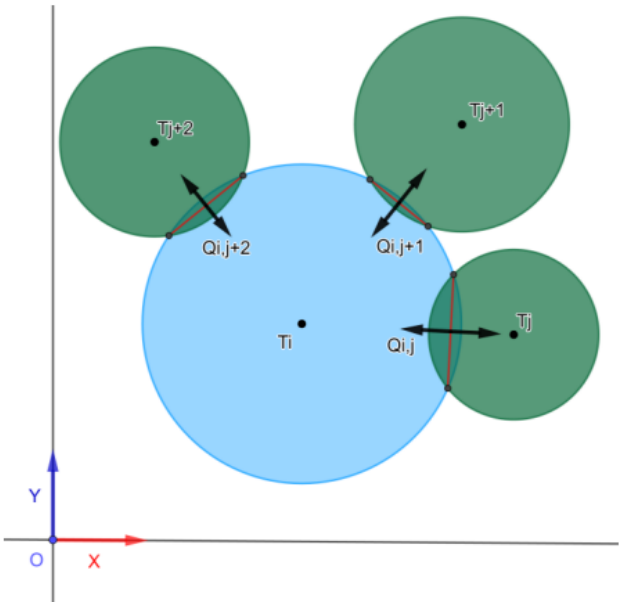


Figure II.5: Contact and heat exchange between several particles

In the case of a medium that contains many molecules that have the same physical and chemical properties, in order to calculate the final temperature of the medium, we first identify the molecules in contact with each other because heat exchange between the molecules requires that they be in contact. Then we calculate the area of contact between the molecules, which is represented by a resulting circle in The ecstasy that occurs when molecules collide with each other, and after you calculate the amount of heat exchanged between the molecules, and by knowing the amount of heat exchanged, the temperature of each molecule can be determine the temperature of each molecule at every moment of time based on knowing its temperature in the initial solution.

CHAPTER III

RESULTS AND DISCUSSIONS

Chapter III

RESULTS AND DISCUSSIONS

III.1 Introduction

This chapter will be dedicated to showcase the software capabilities by considering different cases with gradual increasing complexity. The physical parameters of the study are inspired by the work done by Bodhisattwa Chaudhuri , "Experimentally validated computations of heat transfer in granular materials in rotary calciners" with slight modifications due to the limitations of the calculation power we have. The considered parameters are summarized in the two tables below.

The theory behind the software has been discussed in the previous chapters. However, the hypotheses having been adopted to make the study possible with reasonable calculation capabilities are listed in the next section.

III.2 Hypotheses

The following hypotheses have been adopted to make the study possible:

- The elastic effect is represented by a virtual spring with an equivalent stiffness K
- The elastic losses are modeled by a damping force characterized by the damping coefficient C

- Due to the small size of the particles, there is no variation of the temperature across their volumes. Hence, the temperature within the particle is supposed to be the same.
- Thermal transfer takes place only between particles (not with the cavity walls nor with air)
- Only normal elastic and frictional forces on the particle are considered, the tangential components are to be included in future works
- Curved walls are supposed to be made of distinct linear segments

III.3 The physical parameters are listed in the tables of the next section.

III.3.1 Physical parameters of the study:

As mentioned earlier, the physical parameters of the study are inspired from the work done by Bodhisattwa Chaudhuri , “Experimentally validated computations of heat transfer in granular materials in rotary calciners” with slight modifications due to the limitations of the calculation power we have.

Cavity

Diameter: 0.1524 m

Rotation speed: 10,20,30 rpm

Particles:

Table III.1: Table of parameters employed in DEM simulations

	Notations	Copper	Alumina
Total number of particles	N	8000	20.000
radius of the particles	r	$2(\mathrm{mm})$	$1.0(\mathrm{mm})$
Densityof the particles	ρ	8900 $((\mathrm{kg/m3}))$	3900 $((\mathrm{kg/m3}))$
Specific heat	C_p	$172(J/(kgK))$	$875(J/(kgK))$
Thermal conductivity	k_s	$385W/(mK)$	$36W/(mK)$
Thermal deffusivity	α	$2.5*10^{-7}m^2s^{-1}$	$1.1*10^{-5}m^2s^{-1}$
Cofficient of restitution	e		
particle/particle		0.8	0.8
particle/wall		0.5	0.5
Normal stiffness Cofficient	K		
particle/particle		$6000N/m$	$6000N/m$
particle/wall		$6000N/m$	$6000N/m$
Time Step	$\Delta(s)$	$1-3*10^{-6}s$	$5*10^{-6}s$

Case Studies:

Case 1: The single particle against flat surface

We start first with the simplest case, which consists of a single particle in a free fall interacting with a flat rigid surface. The only variable here is the vertical position of the particle. In figure III.1 we can see the particle of radius 2mm at the initial position inside the 0.05 x 0.0375 m rectangle.

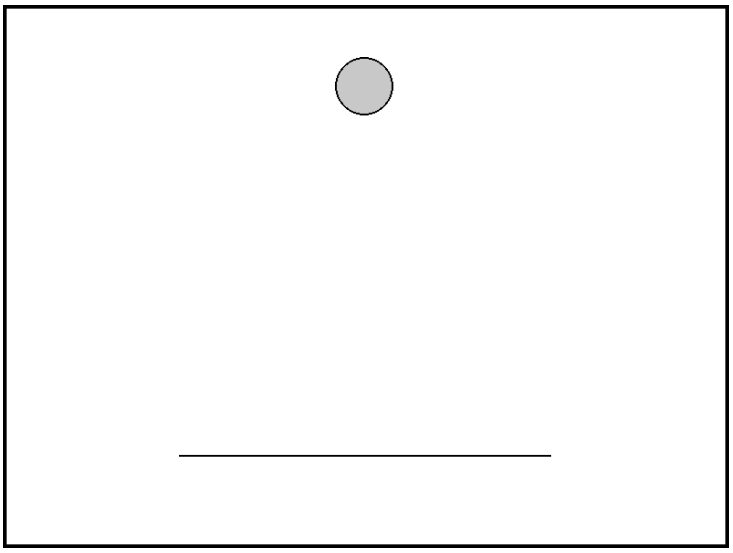


Figure III.1: The single particle against flat surface

A close up of the particle at the moment when it hits the flat surface (see figure III.2), shows clearly how the elastic behavior of the particle is modeled with a virtual interpenetration with that wall.

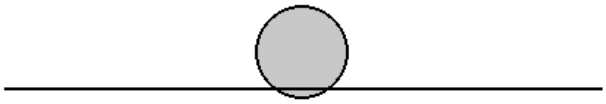


Figure III.2: Close up of the particle at the moment of hit

Figure III.3 shows the y and x positions evolutions with time. As expected only the y varies. We can see clearly the gravity (acceleration) effect on the curve, making the particle decelerates at the maximum height.

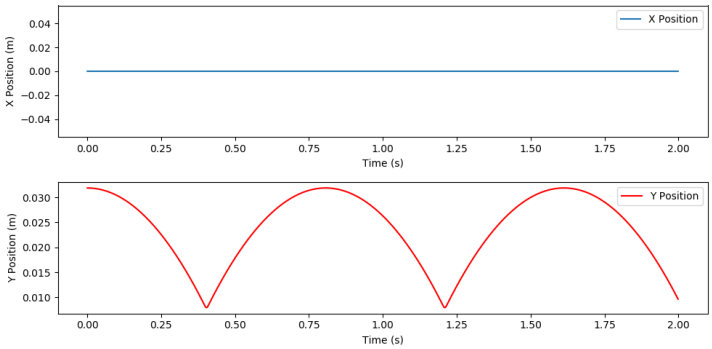


Figure III.3: The y and x positions evolution with time

The absence of damping makes the particle returns to exactly its initial position, which is not realistic. The elastic loss due to the impact against the flat surface is than modeled by introducing a damping force that points always to the opposite direction of the particle speed. The next plot shows the decrease of the particle amplitude due to the introduced damping.

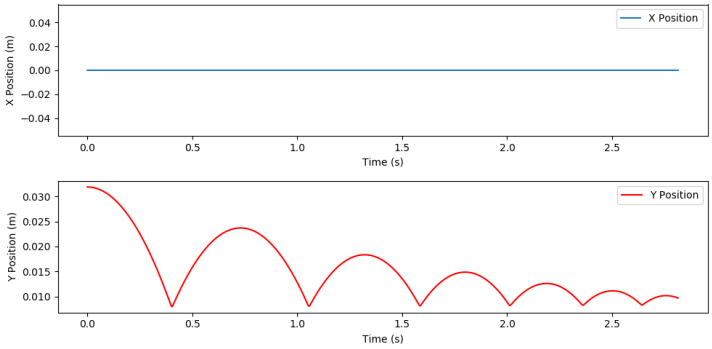


Figure III.4: Decrease of the amplitude due to the damping

Case 2: The single particle against an inclined surface

A simulator with a single degree of freedom can be useful to show how realistic the simulation can be; however, it is with little use beside that. We show the 2D capability of the software by pushing the particle to move in the second direction also (x direction). This is achieved by replacing the flat surface with an inclined one.

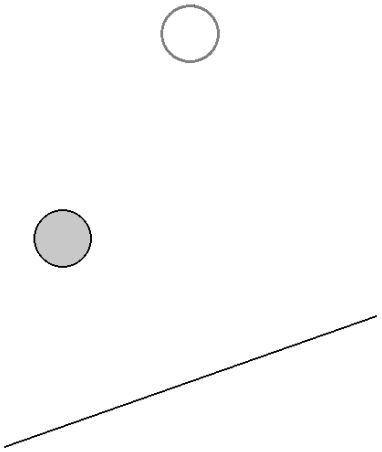


Figure III.5: Deviation of the particle in 2D

Figure III.5 show the deviation of the particle after the percussion with the inclined wall. The Object-oriented programming strategy adopted in the development of the software makes it easy to introduce any wall configuration or to make any surface shape by combining multiple instances (copies) of the object “wall”. This will be detailed more in the last three cases. In the figure III.6 we notice the linear variation by segment of the second degree of freedom (x component).

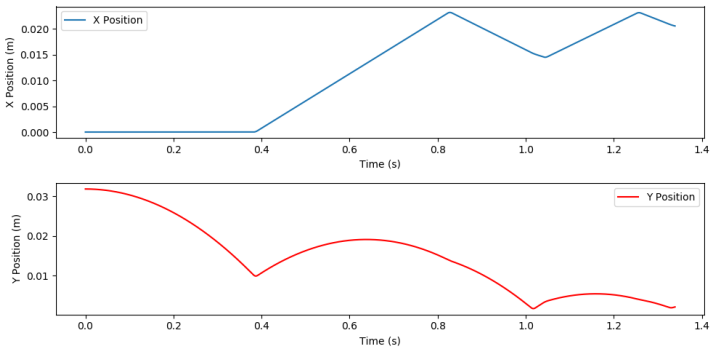


Figure III.6: Variation of the second degree of freedom

Case 3 Multiple particles dynamics

The 3^{rd} case deals with the dynamic interaction of multiple particles without any thermal effect. The initial position of the set of particles with random radii (between 1 and 2 mm) is generated inside a rectangle (figure III.7) taking into account the non-interpenetration between particle

and to fill the maximum space with particles. Mathematically, the problem of the optimum packing of particles with random radii, is a difficult one and no solution has been found yet.

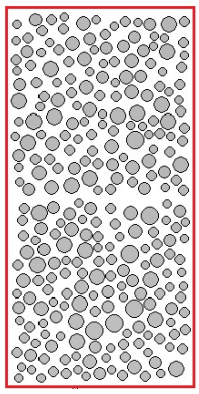


Figure III.7: Initial position of the set of particles

The final triangular shape formed by the particles is generally used to validate any granular particles dynamic code.

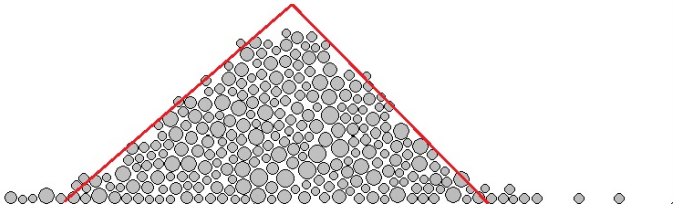


Figure III.8: Final shape formed by the particles at rest

Case 4 The thermal effect between two particles

The next step is to introduce the thermal effect between two particles initially at 100°C and 0°C each. The two particles have the same radius of 2*mm*, are at rest and interpenetrating each other

by 0.2*mm*. This can be insured by setting their positions in a way to make the distance between their centers equals to 3.8*mm*.

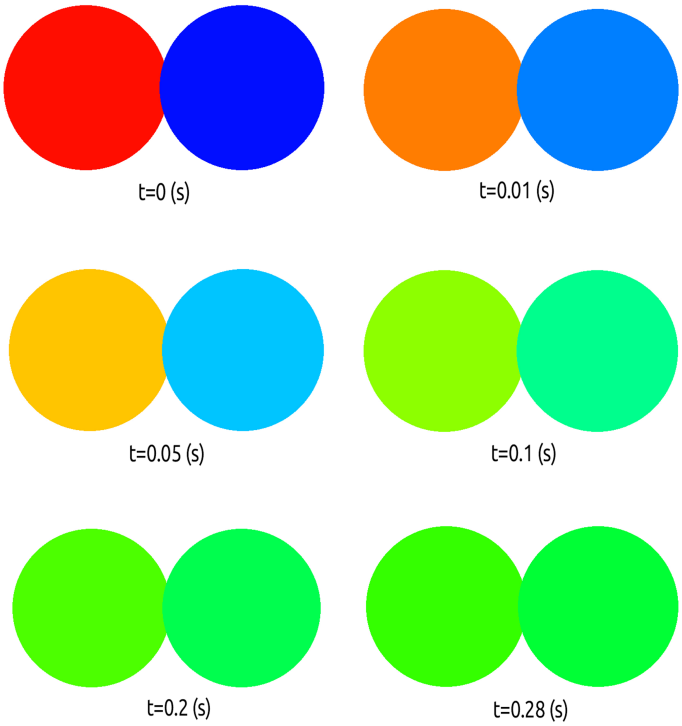


Figure III.9: Temperature evolution of the two particles

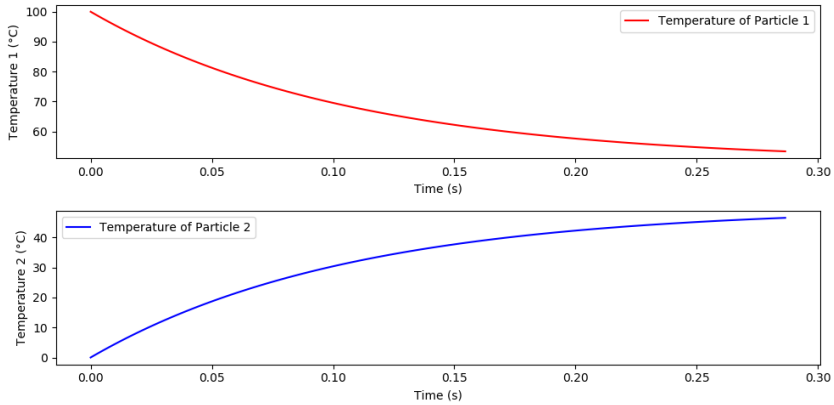


Figure III.10: Temperature evolution of the two particles

In figures III.9 and III.10 we notice that the particles temperatures converge to 50°c which is the average temperature between the two, which makes perfect sense since they have the same physical properties. Now that both the particle's dynamics as well as the transient thermal effect have been tested, in the next cases we couple everything in more elaborate situations.

Case 5 Multiple particles dynamics with thermal effect

The first coupled case deals with the simulation of the free fall of a set of particles initially packed in a rectangular form, then freed to fall toward a flat surface.

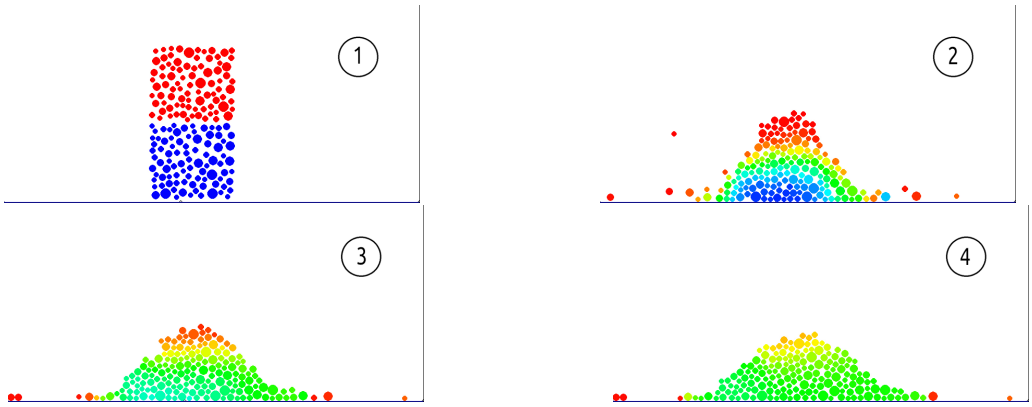


Figure III.11: Temperature and positions evolution

Figure III.11 shows the evolution of the grain positions as well as their temperatures. The triangular shape formed by the particles at rest appears again accompanied with the gradual thermal diffusion. In the next two cases we will simulate areal situation by trying to replicate the experimental setup by [**chaudhuri2010experimentally**] .

Case 6 Smooth cavity in rotation

In [**chaudhuri2010experimentally**] the author describes the use of experiments (figure III.12) to examine flow, mixing, and mass and heat transport in rotary calciners. The physical parameters of the study have been described previously in the 3rd paragraph.

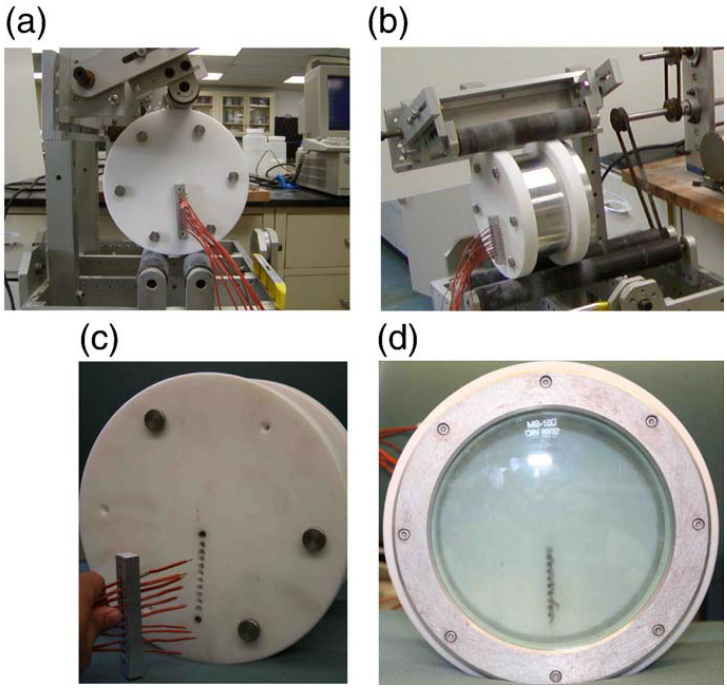


Figure III.12: Experimental setup [**chaudhuri2010experimentally**]

The simulation of half rotation of the container at a speed of 5e-4 rad/s with 214 particles of random radii needs around 1hour of run time on an Intel(R) Core(TM) i7-6600U CPU (2.60GHz 2.81 GHz) with 16.0 Go of RAM running on a 64 bits Windows 10.

The first configuration studied is that of a smooth container (internally), the particles move freely inside it under the effect of its rotation.

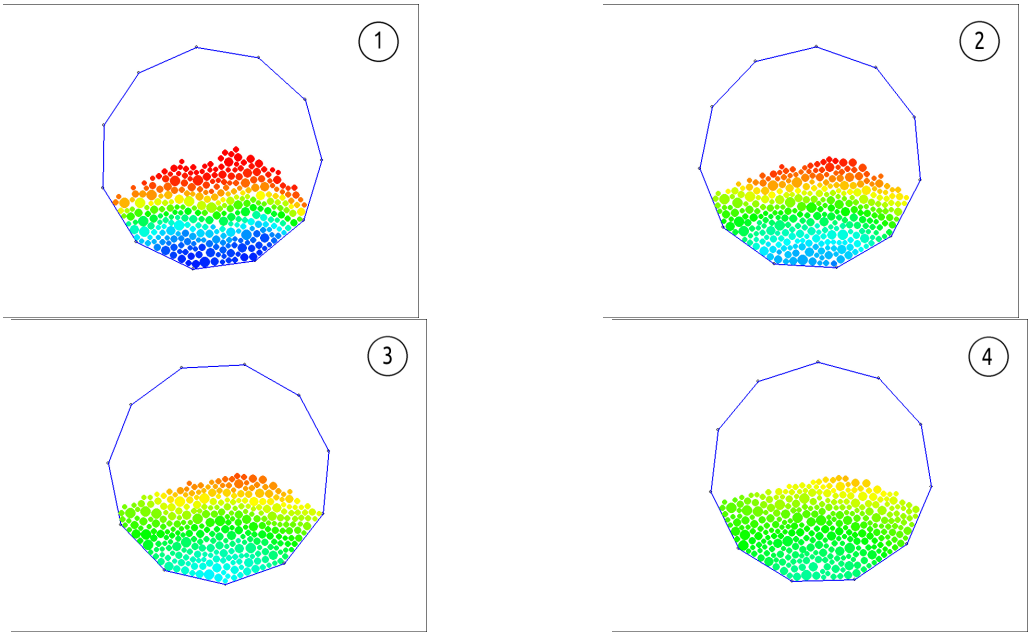


Figure III.13: Particles inside the smooth container

The software developed in this study is capable of importing automatically the container shape from any 2D SVG file. The paths are automatically converted into “wall” objects, which are grouped under a the “Cavity” Class (or object). The “wall” object is written to have the capability to interact with any particle in any situation.

Figure III.13 shows the evolution of the particles positions as well as their temperature inside the smooth container as it rotates. We notice little influence of the cavity rotation as the particles rotates around their selves without changing positions.

Case 7 Cavity with rectangular baffles in rotation

To push the particles to move, a set of L-Shaped flights baffles are added to the container. They are distributed evenly as shown in figure III.14. The geometry of the container is imported automatically (without any user intervention) from an SVG file made using Inkscape. Figure

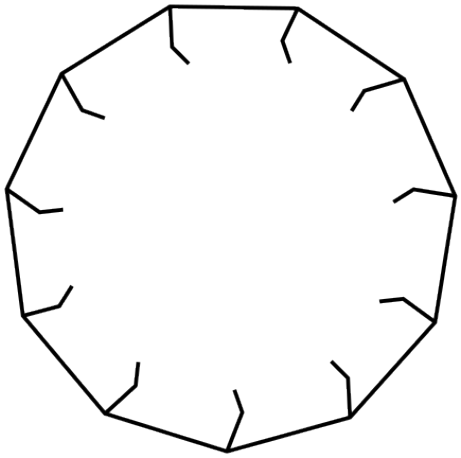


Figure III.14: Container with L-shaped flights baffles

III.15 shows the evolution of the particles positions as well as their temperature inside the modified container as it rotates. We notice huge impact of the introduction of the L-shaped baffles.

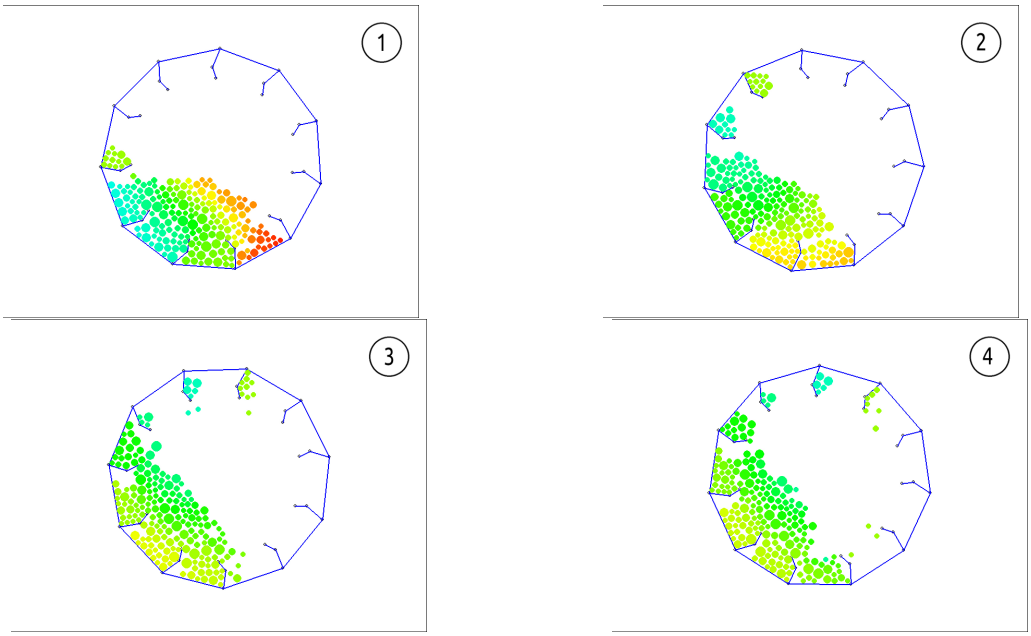


Figure III.15: Particles inside the container with L-shaped flights baffles

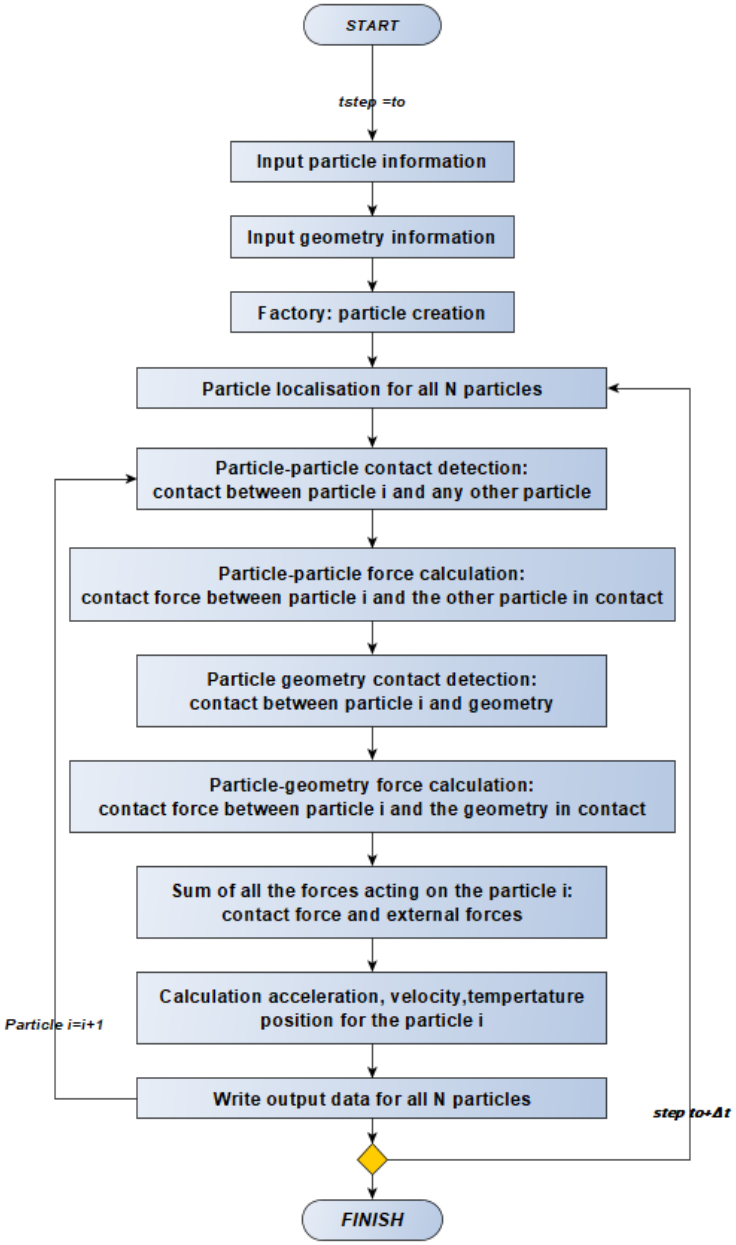


Figure III.16: DEM numerical algorithm

CONCLUSIONS AND PROSPECTS

CONCLUSIONS AND PROSPECTS

The aim of this work being the initiation of the development of a general software based on the discrete element method that takes also the thermal conductivity, adopted approach an "Object Oriented Programming" technique which allows a great flexibility in terms of modularity, expansion and maintenance. We have chosen Python as the programming language due to the availability of a comprehensive set of libraries like the Matplotlib for plotting. The easiness of programming in Python makes it ideal as a drafting tool. After a brief literature review about the discrete element method (DEM), its development and the granular media modeling in general, we exposed the main mathematical formulation related both to the granular mechanical dynamics as well as the heat transfer. To show the capabilities of the developed solution, 8 case studies were exposed in a dedicated chapter. The cases get sophisticated gradually, starting from a simple free fall of a single particle and finishing with a complex granular mixing model in a cylindrical cavity inspired from experimental studies from the literature. For any future work, we propose first to translate the programs into a lower-level programming language such as $C++$ for more control on the memory and to gain more speed. We propose also to add a Graphical User Interface for more flexibility. This can be achieved using Python libraries like Tkinter, by mixing languages or by rewriting the codes entirely using a visual programming language. An interesting idea that can reduce the complexity of modeling the interaction with the flat walls is to model them using "glued" particles.

Appendix A

Annexe A

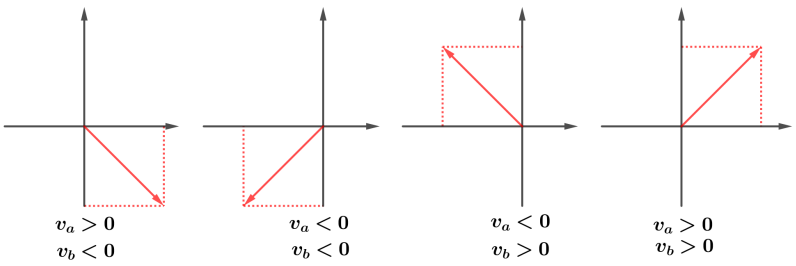


Figure A.1: the four cases of the position of a vector in the 2D quadrants

$$\sum F = m\ddot{x}$$

$$-mg + kx - c\dot{x} = m\ddot{x}$$

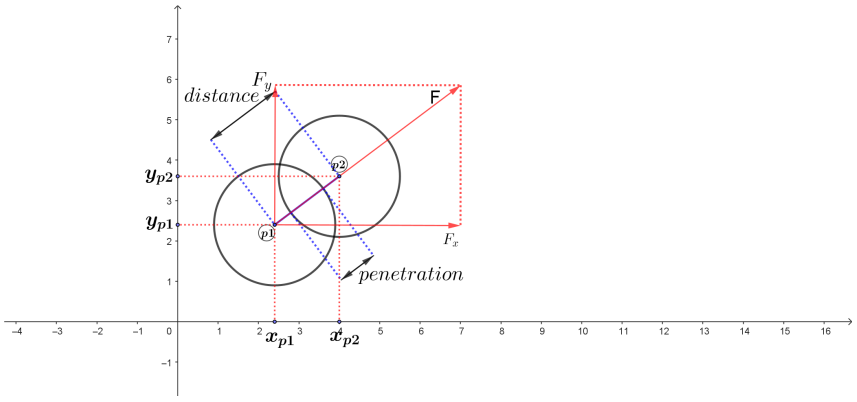


Figure A.2: geometric representation of particle-particle contact

$$\text{distance } = \sqrt{\left(x_{p2} - x_{p1}\right)^2 + \left(y_{p2} - y_{p1}\right)^2}$$

$$\text{Penetration } = 2r - \text{ distance}$$

$$\alpha = \cos^{-1}\left(\frac{x_{p2} - x_{p1}}{\text{distance}}\right)$$

$$F = \text{ Penetration } * k$$

$$\begin{cases} F_x = F\cos(\alpha) - CV_x & \text{When there is perestration} \\ F_y = F\sin(\alpha) - CV_y \end{cases}$$

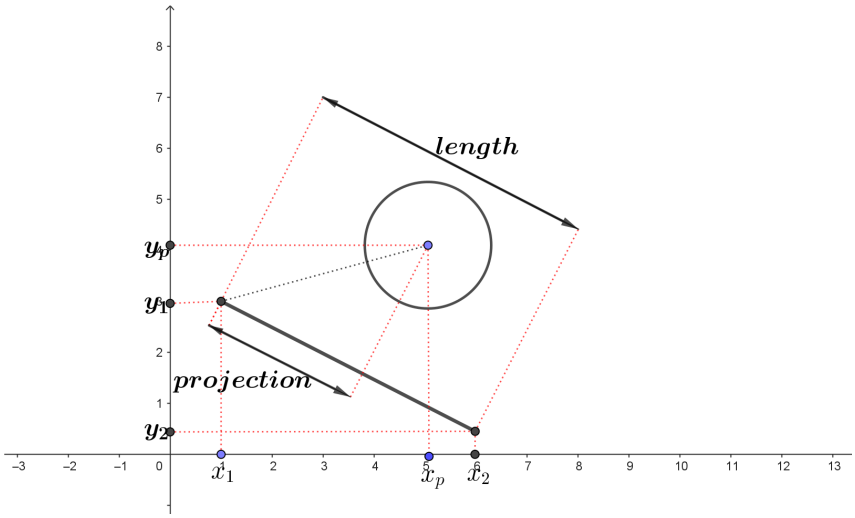


Figure A.3: identification of geometric variables

$$\text{length } = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

$$\text{projection } = \frac{(x_p - x_1) * (x_2 - x_1) + (y_p - y_1) * (y_2 - y_1)}{\text{length}}$$

Projection < 0

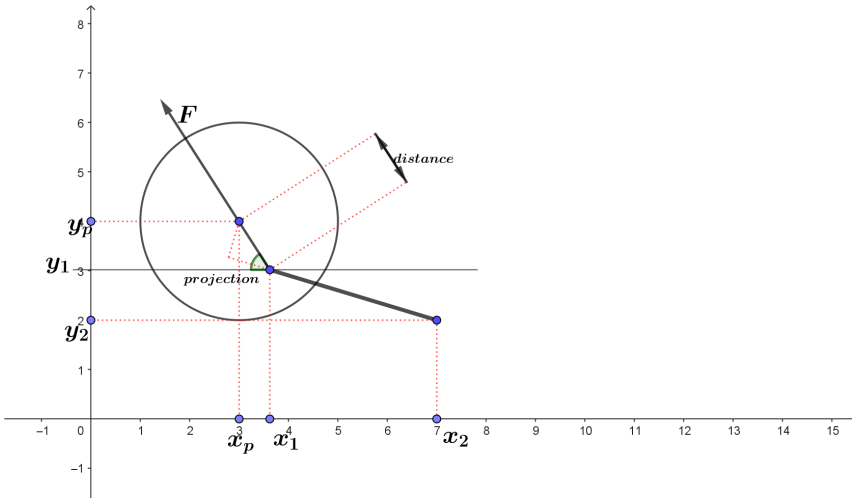


Figure A.4: geometric representation of the extreme contact case on the left

$$distance = \sqrt{(x_p - x_1)^2 + (y_p - y_1)^2}$$

$$Penetration = r - distance$$

$$\alpha = \tan^{-1}\left(\frac{y_p - y_1}{x_p - x_1}\right) \textit{we must consider the cases}$$

$$F = \text{ Penetration } * k$$

$$\begin{cases} F_x = F\cos(\alpha) - CV_x \\ F_y = F\sin(\alpha) - CV_y \end{cases}$$

Projection $>$ length

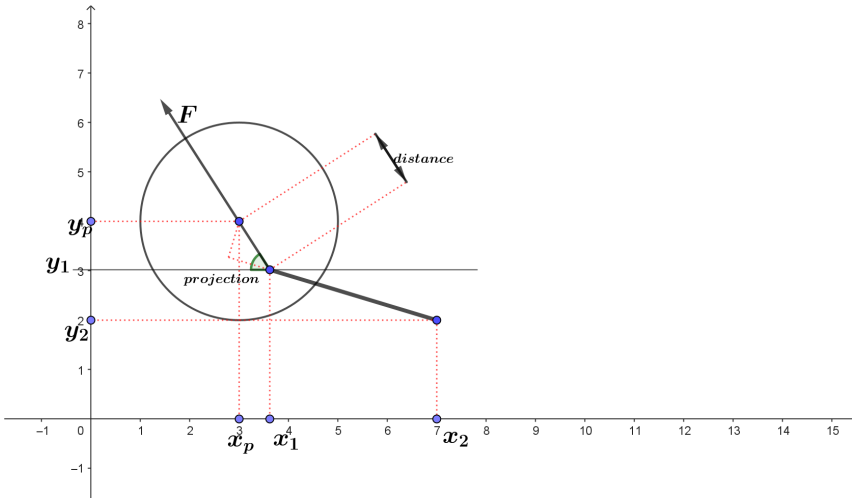


Figure A.5: geometric representation of the extreme contact case on the righ

$$distance = \sqrt{(x_p - x_1)^2 + (y_p - y_1)^2}$$

$$Penetration = r - distance$$

$$\alpha = \cos^{-1}\left(\frac{y_p - y_2}{x_p - x_2}\right)$$

$$F = k + Penetration$$

$$\begin{cases} F_x = F\cos(\alpha) - CV_x \\ F_y = F\sin(\alpha) - CV_y \end{cases}$$

$0 \leq projction \leq lngth$

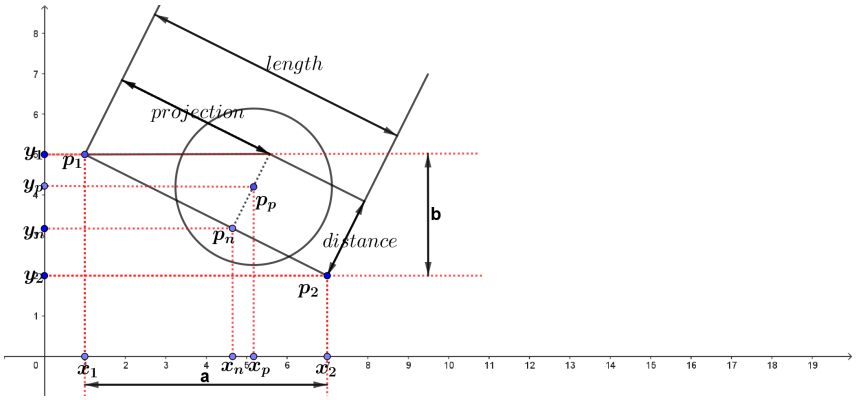


Figure A.6: geometric representation of the general case

geometric representation of the general case $x_2 - x_1 = \gamma$

$y_2 - y_1 = \beta$

composants of the vctor $\vec{P_1P_2}$

How we get $(*)$

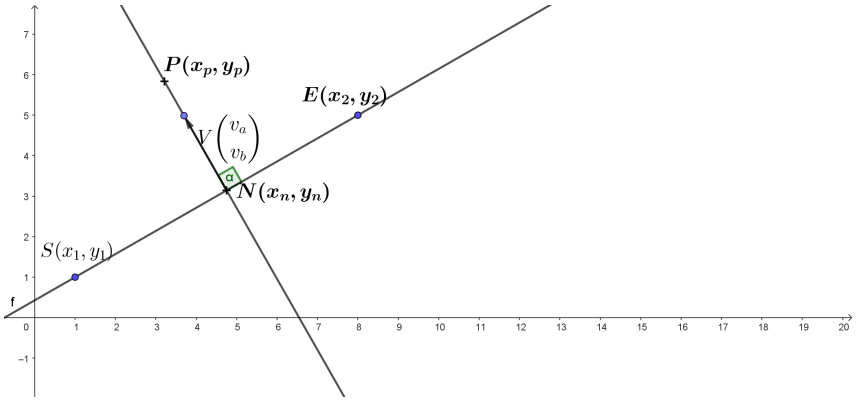


Figure A.7: vector representation of the general case

The equation of the line (SE) (that supports the wall segment) is given by :

$$y = \left(\frac{y_2 - y_1}{x_2 - x_1}\right)x + \left(\frac{y_1x_2 - y_2x_1}{x_2 - x_1}\right) \; or \; \frac{x - x_1}{x_2 - x_1} = \frac{y - y_1}{y_2 - y_1}$$

The vector $\vec{v}$ perpendicular to the line (SE) has the components

$$\begin{cases} v_a = (y_2 - y_1) \\ v_b = -(x_2 - x_1) \end{cases} or \begin{cases} v_a = -(y_2 - y_1) \\ v_b = (x_2 - x_1) \end{cases}$$

The equation of the line passing by N and parallel to $\vec{v}$ is given by:

$$\frac{x-x_p}{y_2-y_1}=\frac{(y-y_p)}{-(x_2-x_1)}\ or\ \frac{x-x_p}{y_2-y_1}=\frac{-(y-y_p)}{(x_2-x_1)}$$

Which is the same Since N belongs to both lines$\Rightarrow$

$$\begin{cases} \frac{x_n-x_1}{x_2-x_1}=\frac{y_n-y_1}{y_2-y_1} \\ \frac{x_n-x_p}{y_2-y_1}=\frac{y_n-y_p}{-(x_2-c_1)} \end{cases} \ we\ note \begin{cases} \gamma=x_2-x_1 \\ \beta=y_2-y_1 \end{cases}$$

$$\begin{cases} \frac{x_n-x_1}{\lambda}=\frac{y_n-y_1}{\beta} \\ \frac{x_n-x_p}{\beta}=\frac{y_n-y_p}{\lambda} \end{cases}$$

$$\Rightarrow \begin{cases} x_n-x_1=\frac{\gamma}{\beta}(y_n-y_1).....(1) \\ x_n-x_p=\frac{\beta}{\gamma}(y_n-y_p).....(2) \end{cases}$$

(1)-(2) gives:

$$x_p-x_1=\left(\frac{\gamma}{\beta}-\frac{\beta}{\gamma}\right)y_n+\frac{\beta}{\gamma}y_p-\frac{\gamma}{\beta}y_1$$

$$\Rightarrow \mathrm{y}_n=\frac{\left(x_p-x_1\right)-\left(\frac{\beta}{\gamma}y_p-\frac{\gamma}{\beta}y_1\right)}{\left(\frac{\gamma}{\beta}-\frac{\beta}{\gamma}\right)}.....(3)$$

from (1)we get : $x_n=\frac{\gamma}{\beta}(y_n-y1)+x_n$

$$\begin{cases} y_n=\frac{\left(x_p-x_1\right)+\left(\frac{\gamma*y_1}{\beta}+\frac{\beta*y_p}{\gamma}\right)}{\frac{\gamma}{\beta}+\frac{\beta}{\gamma}} \\ x_n=-\frac{\beta*y_n}{\gamma}+\frac{\beta*y_p}{\gamma}+x_p \end{cases}$$

$$\text{distance} = \sqrt{(x_p - x_n)^2 + (y_p - y_n)^2}$$

$$Penetration = r - distance$$

$$\alpha = \cos^{-1}\left(\frac{x_p - x_n}{distance}\right)$$

F=k+ Penetration

$$F_x = F\cos(\alpha) - CV_x$$

$$F_y = F\sin(\alpha) - CV_y$$

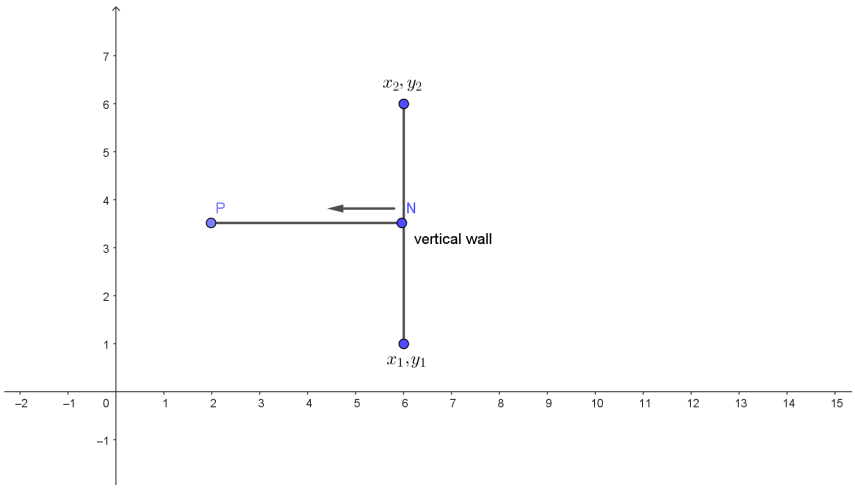


Figure A.8: special case when the wall is vertical

$if\ x_1 = x_2$

$$\begin{cases} y_n = y_p \\ x_n = x_1 \end{cases}$$

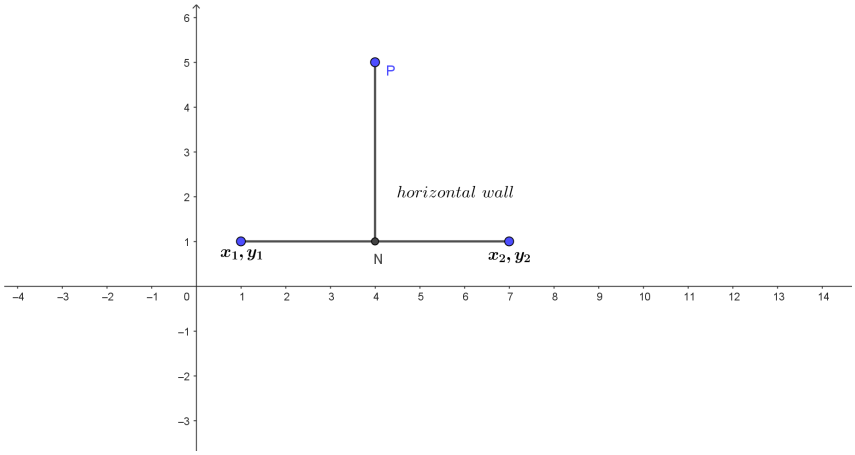


Figure A.9: special case when the wall is horizontal

$if\ y_1 = y_2$

$$\begin{cases} y_n = y_1 \\ x_n = x_p \end{cases}$$

Appendix B

Annexe B

BMC

BUSINESS MODEL CANVAS

TechnoFoster

نموذج مخطط الأعمال للمشاريع الخاصة بالقرار 1275

Presentation 2024

المحتوى

ما هو مشروعك؟

في هذا العمل طورنا برنامجا هدفه الرئيسي دراسة و تطوير أداة تعتمد على طريقة العناصر المنفصلة (. DEM)
تم تطوير البرنامج بإعتماد لغة python, البرنامج يعتبر الأول من نوعه من حيث الوظيفة التي يقوم بها بحيث يقوم بمحاكات و دراسة التطورات ,الحركية والحرارية في آن واحد على عكس باقي البرامج التي تتفرد بإحدى الدراسات و بذالك أكدنا أن DEM هي الطريقة الأنسب لمعالجة إنتقال الحرارة في الوسائط الحبيبية.

لماذا مشروعك؟

بسبب أن الشركات الصناعية التي تعمل مع عمليات تشمل المواد الحبيبية (الصيدلانية والكيميائية ومعالجة الأغذية والتلبيد بالليزر الانتقائي (SLS) الطباعة ثلاثية الأبعاد، الهندسة المدنية).

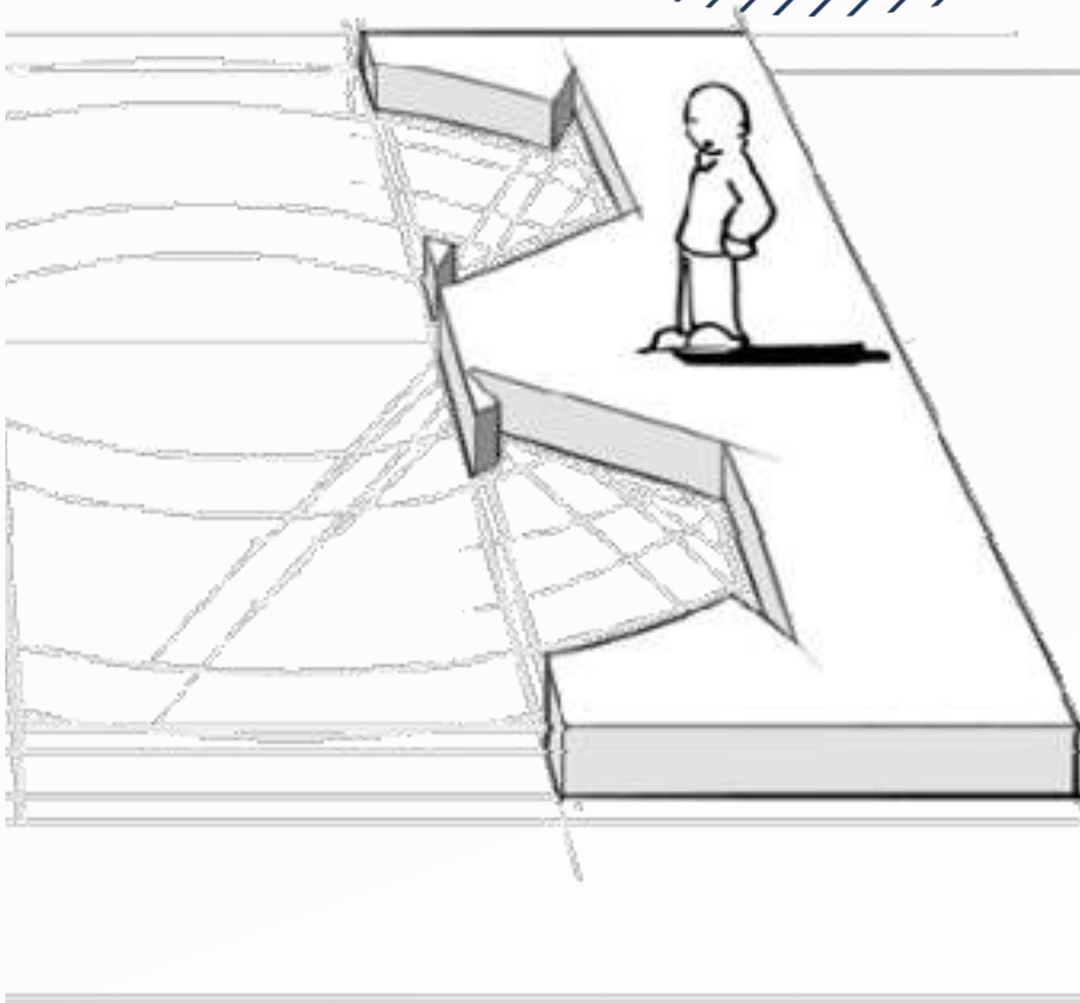
- عدم وجود برنامج يحاكي كل التغيرات في ان واحد
- صعوبة التحكم بدرجة الحرارة في المسحوق

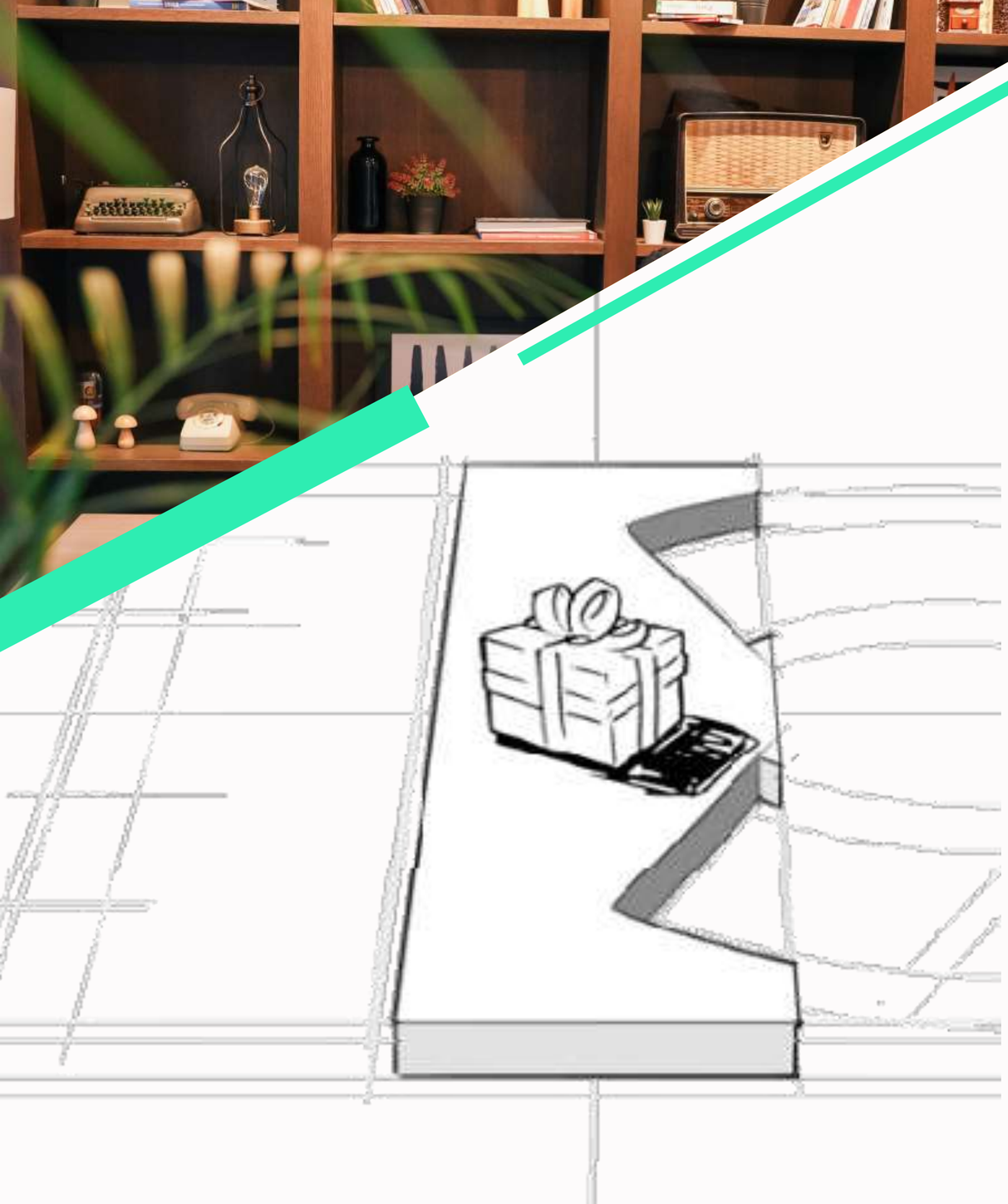
القيمة المضافة

- التقاط تفاعلات الجسيمات المعقدة وآليات نقل الحرارة التي يصعب نمذجتها بالطرق التقليدية
- تخفيض الوقت والتكلفة
- **سهولة الاستخدام** :ستكون الأداة سهلة الاستخدام مع واجهة مستخدم رسومية ووثائق شاملة.
- **قابلية التمديد** :ستكون الأداة قابلة للتمديد لتضمين ميزات جديدة في المستقبل
- فهم أفضل لانتقال الحرارة مثل طباعة ثلاثية الأبعاد SLSو تحسين جودتها

شرائح العملاء أو الزبائن Customer Segments

- باحثون في المجالات الهندسية يدرسون نقل ديناميكية الجسيمات ونقل الحرارة في المواد الحبيبية.
- الشركات الصناعية التي تعمل مع عمليات تشمل المواد الحبيبية الصيدلانية، والكيميائية، والتلبيد بالليزر الانتقائي SLS 3D Printingالطباعة ثلاثية الأبعاد، والهندسة المدنية.)





القيمة المقترحة

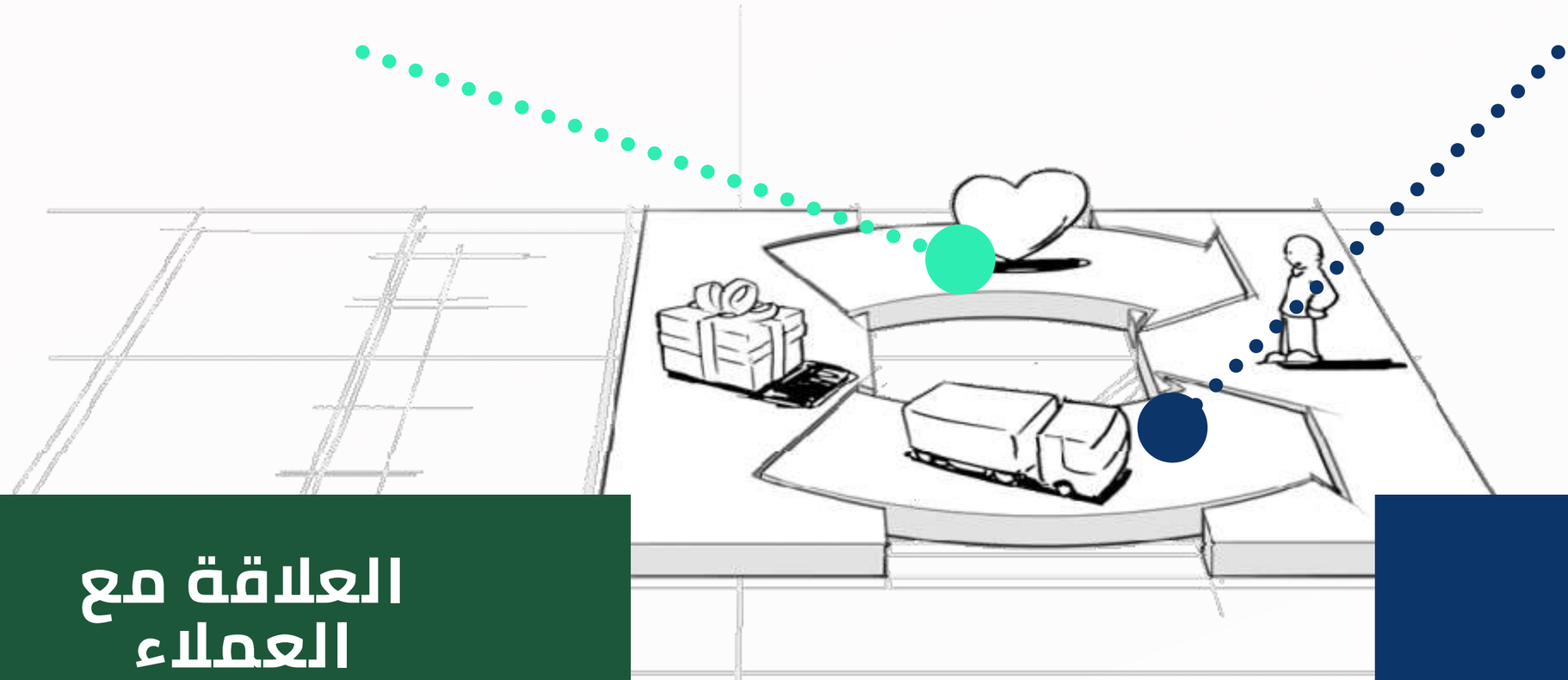
- يوفر طريقة أكثر دقة وكفاءة لمحاكاة انتشار الحرارة في الوسائط الحبيبية مقارنة بالطرق التقليدية.
- تخفيض الوقت والتكلفة
- محاكاة نقل الحرارة في الوسائط الحبيبية ، مما يلغي الحاجة إلى تجارب فيزيائية باهظة الثمن.
- التقاط تفاعلات الجسيمات المعقدة وآليات نقل الحرارة التي يصعب نمذجتها بالطرق التقليدية.
- تحسين العمليات الصناعية التي تتضمن مواد حبيبية عن طريق محاكاة سيناريوهات مختلفة والتنبؤ بسلوك نقل الحرارة

- المؤتمرات والمنشورات الأكاديمية
- أسواق البرمجيات الهندسية
- المبيعات المباشرة للشركات الصناعية

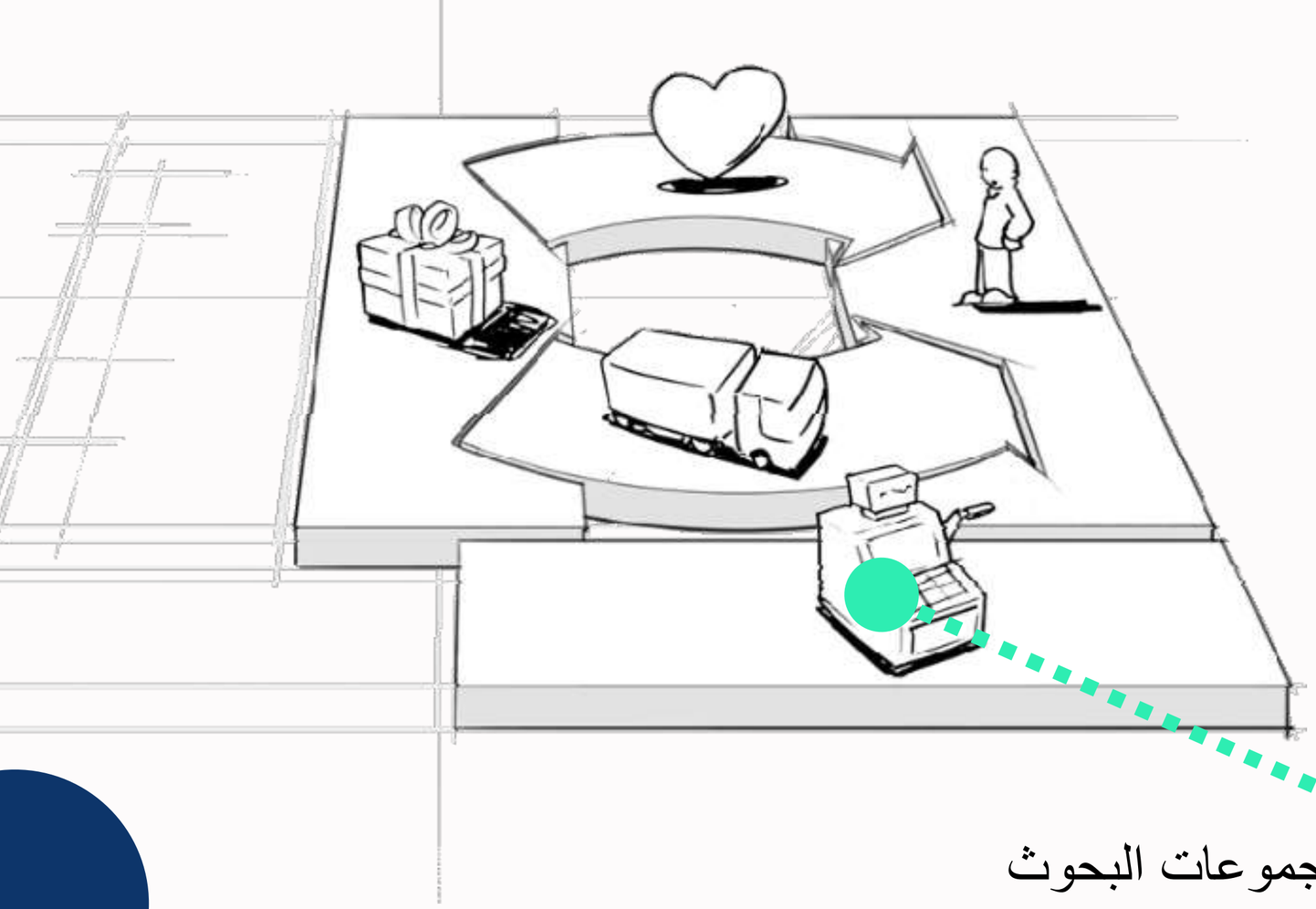
القنوات

- توفير الدعم التقني والتدريب للمستعملين
- عرض خيارات التكييف مع احتياجات بحثية أو صناعية محددة
- الحفاظ على مجتمع نشط على الإنترنت للمستخدمين لتبادل الخبرات والمعارف

العلاقة مع العملاء



مصادر الدخل (الإيرادات)

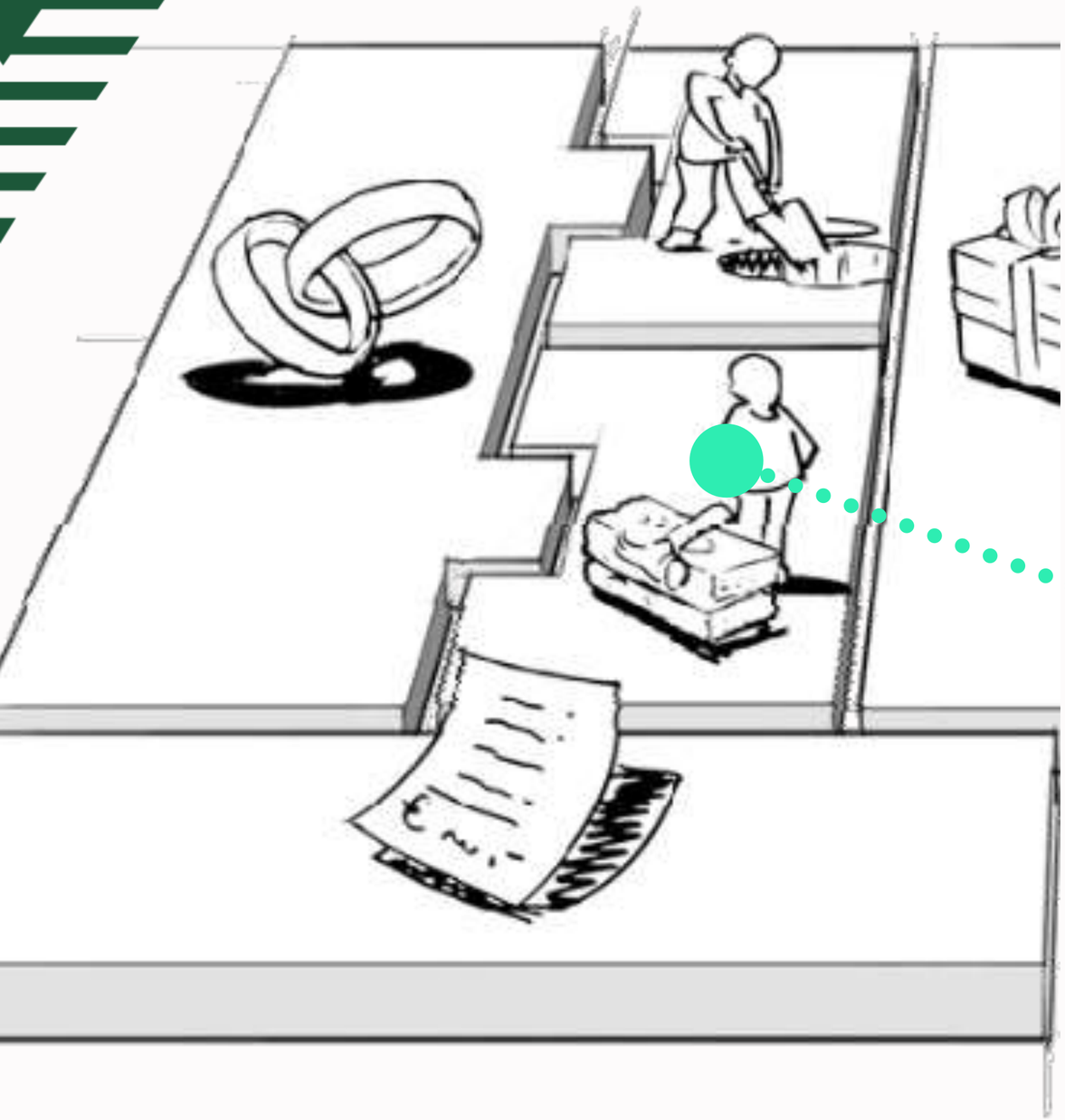


- بيع تراخيص البرمجيات للمؤسسات الأكاديمية ومجموعات البحوث
- تقديم خدمات محاكاة قائمة على السحابة مع تسعير الدفع لكل استخدام
- تقديم خدمات استشارية للشركات الصناعية

المهام (الأنشطةُ) الأساسية

- تحسين وتحديث برنامج DEMباستمرار
- تطوير واجهة سهلة الاستخدام تسويق البرامج وترويجها لاستهداف الجماهير
- توفير الدعم التقني والتدريب للمستعملين

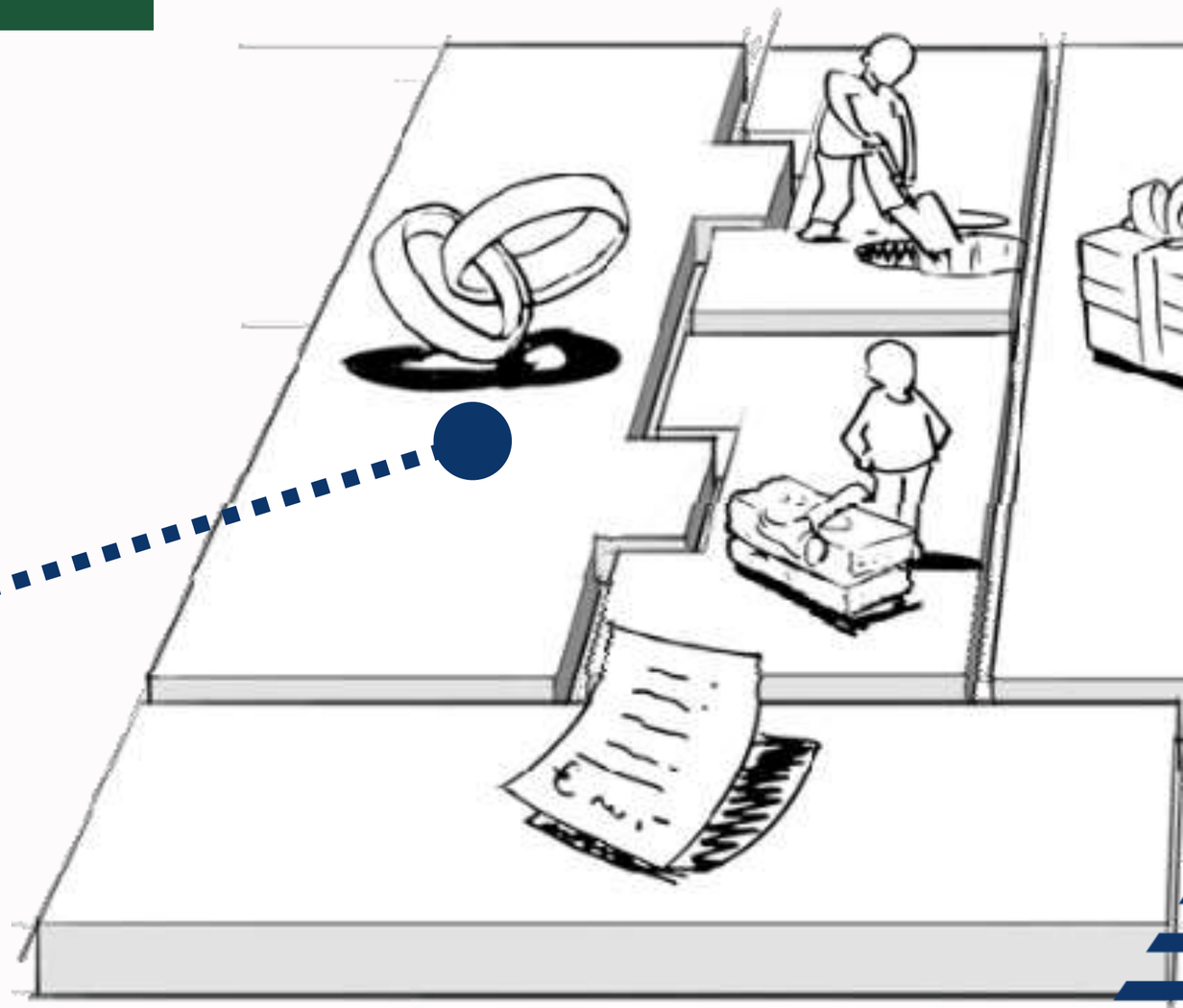
الموارد الرئيسية



- موارد حوسبة عالية الأداء لإجراء عمليات محاكاة
- فريق ذو خبرة في البرمجة و الحوسبة العلمية

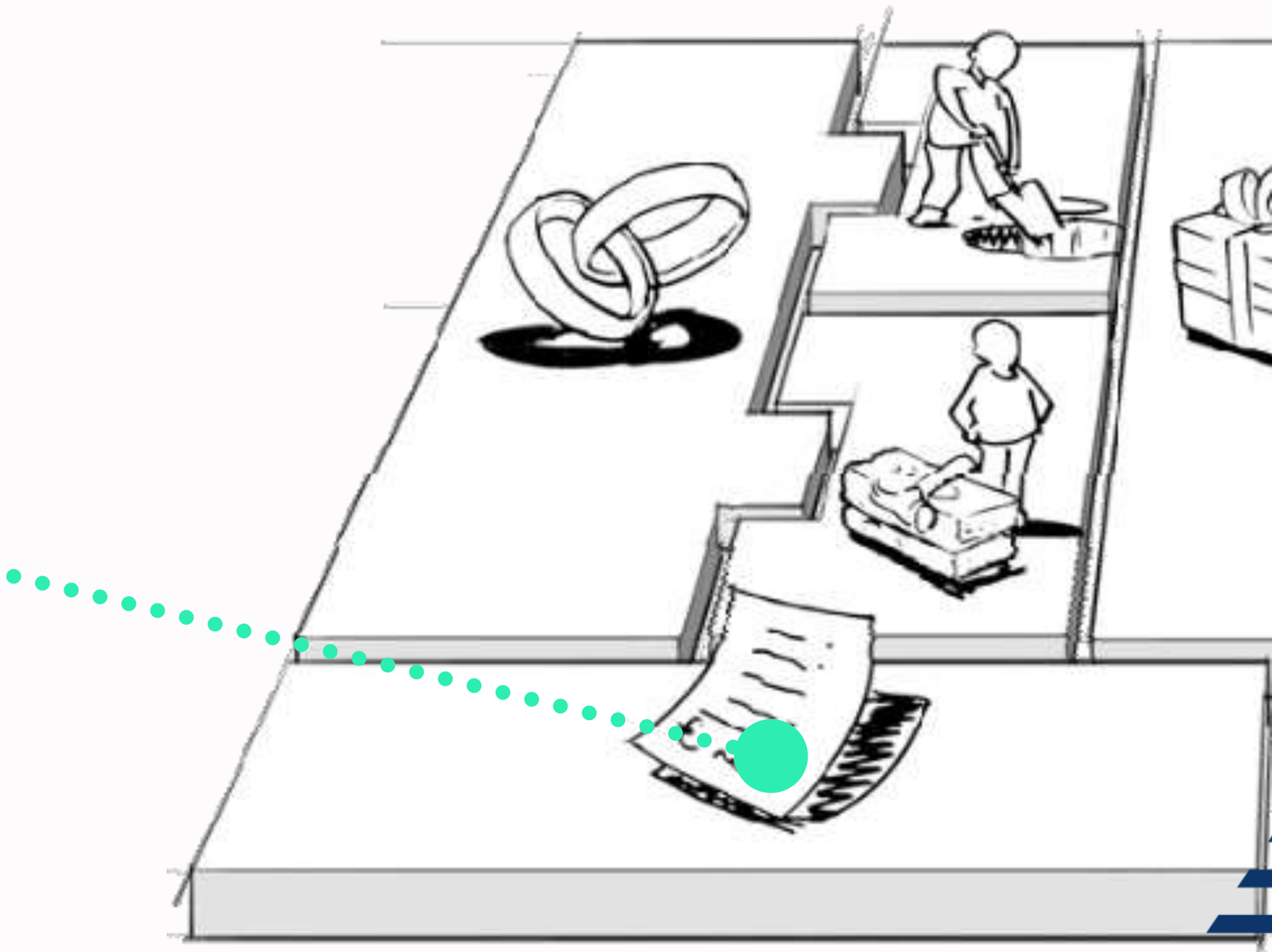
الشركاء الرئيسيَّين

- التعاون مع الباحثين الأكاديميين لتطوير الكود والتحقق من صحته
- شراكة مع شركات البرمجيات الهندسية للتوزيع
- العمل مع قادة الصناعة لتحديد احتياجاتهم الخاصة وتلبيتها



هيكل التكاليف

- تكاليف تطوير وصيانة البرمجيات
- الموارد الحاسوبية العالية الأداء
- نفقات التسويق والمبيعات
- دعم العملاء



Business Model Canvas

Desianed for:	Desianed bu:	Date:	Version:

Customer Segments

- باحثون في المجالات الهندسية يدرسون نقل الحرارة في المواد الحبيبية.
- الشركات الصناعية التي تعمل مع
- عمليات تشمل المواد الحبيبية (الصيدلانية، والكيميائية، وتجهيز
- الأغذية، والتلبيد بالليزر الانتقائي
- والطباعة ثلاثية الأبعاد، والهندسة
- المدنية).

Customer Relationships

- توفير الدعم التقني والتدريب للمستعملين
- عرض خيارات التكييف
- مع احتياجات بحثية أو صناعية محددة
- الحفاظ على مجتمع نشط على الإنترنت
- للمستخدمين لتبادل الخبرات والمعارف

Channels

- المؤتمرات والمنشورات الأكاديمية
- أسواق البرمجيات الهندسية
- المبيعات المباشرة للشركات الصناعية

Value Propositions

- يوفر طريقة أكثر دقة وكفاءة لمحاكاة انتشار الحرارة في الوسائط الحبيبية مقارنة بالطرق التقليدية.
- تخفيض الوقت والتكلفة
- محاكاة نقل الحرارة في الوسائط الحبيبية ، مما يلغي الحاجة إلى تجارب فيزيائية باهظة الثمن.
- التقاط تفاعلات الجسيمات المعقدة وآليات نقل الحرارة التي يصعب نمذجتها بالطرق التقليدية.
- تحسين العمليات الصناعية التي تتضمن مواد حبيبية عن طريق محاكاة سيناريوهات مختلفة والتنبؤ بسلوك نقل الحرارة.

Key Activities

- تحسين وتحديث برنامج DEMباستمرار
- تطوير واجهة سهلة الاستخدام
- تسويق البرامج وترويجها لاستهداف الجماهير
- توفير الدعم التقني والتدريب للمستعملين

Key Resources

- تم تطوير برنامج DEM باستخدام Python
- موارد حوسبة عالية الأداء لإجراء عمليات المحاكاة
- فريق ذو خبرة في الميكانيكا الحبيبية ونقل الحرارة والحوسبة العلمية

Key Partners

- التعاون مع الباحثين الأكاديميين
- لتطوير الكود والتحقق من صحته
- شراكة مع شركات البرمجيات الهندسية للتوزيع
- العمل مع قادة الصناعة لتحديد احتياجاتهم الخاصة وتلبيتها

Revenue Streams

- بيع تراخيص البرمجيات للمؤسسات الأكاديمية ومجموعات البحوث
- تقديم خدمات محاكاة قائمة على السحابة مع تسعير الدفع لكل استخدام
- تقديم خدمات استشارية للشركات الصناعية

Cost Structure

- تكاليف تطوير وصيانة البرمجيات
- الموارد الحاسوبية العالية الأداء
- نفقات التسويق والمبيعات
- دعم العملاء

TechnoFoster

Contact Us

+213 46 25 61 33

incubator@univ-tiaret.dz

fb.com/techno.foster.incubator

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SUMMARY

This thesis aims to develop a general software using the discrete element method (DEM) that incorporates thermal conductivity. The project employs Object Oriented Programming (OOP) in Python, chosen for its modularity, ease of use, and extensive libraries such as Matplotlib for plotting. The thesis begins with a literature review on DEM and granular media modeling, followed by an exposition of the mathematical formulations for granular mechanical dynamics and heat transfer. The software's capabilities are demonstrated through eight progressively complex case studies, culminating in a granular mixing model.

RESUMES

Cette thèse vise à développer un logiciel général utilisant la méthode des éléments discrets (DEM) qui intègre la conductivité thermique. Le projet emploie la programmation orientée objet (POO) en Python, choisi pour sa modularité, sa facilité d'utilisation et ses bibliothèques étendues telles que Matplotlib pour le traçage. La thèse commence par une revue de la littérature sur la DEM et la modélisation des milieux granulaires, suivie d'une exposition des formulations mathématiques pour la dynamique mécanique des granulaires et le transfert de chaleur. Les capacités du logiciel sont démontrées à travers huit études de cas de complexité progressive, culminant avec un modèle de mélange granulaire.

ملخص

تهدف هذه الأطروحة إلى تطوير برنامج عام باستخدام طريقة العناصر المنفصلة (*DEM*) مع اعتبار النقل الحراري كذلك. يستخدم المشروع تقنية البرمجة (*OOP*) لمرونتها وقوة تمديدها اما لغة البايثون فلتوفره على مكتبات كثيرة وقوية مثل مكتبة *Matplotlib* للرسم البياني. تبدأ الأطروحة بمراجعة الأدبيات حول *DEM* ونمذجة الوسائط الحبيبية، تليها عرض الصيغ الرياضية لديناميكيات الميكانيكا الحبيبية وانتقال الحرارة. يتم عرض قدرات البرنامج من خلال ثماني دراسات تتزايد في التعقيد، وتبلغ ذروتها بنموذج خلط حبيبي.