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SIMULATION ROUTINE IN YADE (FREE ACCESS) FOR GRAIN FLOW IN LARGE SILOS USING DISCREET ELEMENT METHOD (DEM)

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Abstract: Granular systems exhibit behaviors not predicted in fluid mechanics or solid mechanics. Although in the past they have been treated in one field or another, in recent decades a whole new theoretical field has been developed to analyze phenomena that were known, but not well described in the literature. In Silos Movement, several situations can occur, such as in the flow of grains in an hourglass that, unlike liquids, the pressure on the walls is not proportional to the height. For this reason, when flowing, the grains can form tension arcs, blocking the flow. This flow of grains in silos is a topic of interest to several sectors of the economy. From grain silos in the agroindustry, through the transport of ores in mining to the flow of coal to the steel industry, with this I realized the importance of this topic. The flow characteristics of the grains depend on several factors, such as the shape and composition of the particle, to its mechanical properties. Adding this range of variations and the fact that the granular system is not continuous, its description through computer simulation is more suitable for observing flow behavior. Given this importance, several commercial platforms for monitoring and predicting flows have been developed in recent years, with high-cost licenses. However, there are open source solutions, which are based on the discrete element method, capable of performing large-scale simulations. With this, the present study presents an open code, adapted and tested in Python, using the discrete element method - DEM, with emphasis on the typical application in mining and steel. This code gives the opportunity to, in addition to understanding the routines, adapt them to the scenario in which it will be used.
Keywords: Granular systems, flow, silos, tension arcs.

INTRODUCTION

The beginning of discussions on the dynamics of particulate systems was the pioneering work on sand piles [1]. Based on the results found, a whole theory was created about the behavior and interaction between grains in flow, mobilizing a good part of the Statistical Physics of the time [2]. Thus, several authors have correlated particle dynamics to their situations. We have as an example the study on energy optimization in the flow of grains and ores, demonstrating the importance of studying the dynamics of granular systems [1-5].

Granular materials are agglomerates of solid particles, in which the interaction between the particles occurs by contact forces [2]. Although in many cases these grains are tiny, they are too large to be treated as thermodynamic fluctuations, so these interactions are considerable [6,7]. Furthermore, granular systems are systems far from thermodynamic equilibrium, requiring computer simulation methods to understand their dynamics [8].

Common examples of granular materials are sand, seeds, gravel, cement and ores. These materials are present in several industrial areas, such as the agribusiness, pharmaceuticals, geology, mining and steel. Therefore, its behavior is studied by several research groups all over the world, both for basic research and for applied sciences and engineering.

Brazil is the second largest exporter of iron ore in the world, accounting for values of around R$22 billion in 2019 [9]. In addition, it is also the largest producer of soybeans in the world and the 8th largest producer of steel in the world, being in eighth place in the ranking of producers [10]. Thus, storage and flow of grains (here included soybeans, coal or iron ore pellets) is of strategic importance for the country, as the optimization of parameters can greatly reduce the cost of production and

transport of these items.

The studies are usually done in physical models or through simulations, or a combination of the two approaches, in which physical models are usually used to "calibrate" the computational models [10].

To obtain useful information for industrial processes, the discrete element method (DEM) was used, as these methods allow more realistic approaches and parameter adjustments closer to reality [1,2].

Given the importance of monitoring and simulating the flow of particles, several simulation platforms are available on the market, but their cost, in general, is very high. Thus, research works have used licenses with size restrictions, available for students or restricted to academic use, limiting simulations, since millions or billions of particles are needed for more realistic systems [1,2,11].

Thus, the present study developed a simulation routine for grain flow in silos, with the possibility of simulating large systems using the YADE software, which has a language similar to Python. The advantage is that the codes are available and can be studied, enabling their adaptation, contributing to their development.

MATERIALS AND METHODS

In the present study, YADE (open source) was used as a platform. The platform customization routines are developed in Python. When working with YADE, the importance of contacting Python is even greater, as it was developed using the standard Python syntax for writing programs.

Another important point for the development of the work was the use of the Linux operating system, in question Xubuntu version 18.04 (bionic), because the YADE simulation platform needs this operating system.

The code had as an approach the visible simulation (visual representation) of the simulated materials, in addition to sampling the energies involved in the process. The code was described in the next topic.

DISCUSSION

Several classes of computational methods can be referred to to simulate any process. The choice of this method has more to do with the nature of the problem. For example, to study the heat flow in continuous materials, or even the propagation of mechanical stresses, a method for solving differential equations is used, such as the Finite Element Method (FEM), for example [1-3,12].

In the present study, the fall of generic grains (to be defined by the operator) in silos was simulated. For this, the platform class that uses the Discrete Element Method (DEM) was used to solve the problems [1-4,13]. Very similar to the approach used in Molecular Dynamics, this method defines the equations of motion for a system formed by particles. Each one of them is associated with a position and velocities, as well as the forces that act on it [14,15].

However, the choice to use a DEM platform is due to the fact that the FEM uses finite methods with approximations of results tending to continuity, and this for a considerably large system can make the simulation unfeasible, whereas the DEM, despite a greater loss of information, due to truncation, presents good results in extremely more viable runtime [1,2,15,16].

As considerations, it is defined that most interactions are short-range and are only produced by the contact between particles. In the present case, we only have the elastic forces produced by compression and friction forces between the particles. Particles that do not touch each other do not interact with each other. Thus, interactions between grains

are dissipative due to static friction and inelasticity of collisions [17]. Another fact to be considered is the fact that temperature has no influence, so thermodynamic arguments are not considered [17,18].

Figures 1-3 show the simulation code on a visible scale using the YADE software, to visualize the formation of a grain pile with the possibility of parameter variation.

After executing the code in YADE, three windows are generated. The first one refers to the interaction interface of YADE itself, where you have the possibility to access execution commands, such as start, pause, rewind, view, change the point of view, among other more advanced ones, represented by Figure 4. The second window visualized is the graph where the internal energies of the system will be presented, shown in figure 5. The last one is the visualization window of the grain system itself, figure 6, showing the visual behavior of the grains flowing in the silo.

It can be seen that the geometry chosen for the silo in question was that of a body with a conical base, containing a bottleneck through which the generated grains will flow naturally due to the action of gravity, in addition to the interactions between the grains themselves and with the silo walls.

After the exit, there are walls at the bottom of the cone, creating a limit, because if any of these grains escape, they will fall infinitely, generating unwanted results (tip to avoid outliers).

After starting the simulation, the first action of falling grains can be seen in figure 7.

As the simulation time passes, the movement of the grains continues, until a pile is formed on the plane and all the grains fall, as shown in figure 8.

At this point in the execution of the simulation, the data collection stage ends, resulting in the graph with the sampling of the finalized energies, plotted as shown in figure 9.

To analyze, the list of energies contained in the system, represented in the graph of Figure 9, are:

- Gravitational potential (green);
- Kinetics (red);
- Non-viscous damping (purple);
- Elastic potential (brown);
- Plastic dissipation (pink);
- Unbalanced energy (blue).

The gravitational potential energy is the initial energy of the system, being stored in the particles at the initial moment of the simulation [18]. After starting the simulation, this energy was gradually converted into kinetic energy [1-3,19]. At that moment, there is an increase in kinetic energy and a smoothing in the decrease in gravitational potential energy, as seen in the graph in Figure 9. This can be explained by the deceleration due to the contact of the particles with the silo wall [2,20].

Because of this contact between the particles and the silo wall, an abrupt increase in dissipative energies is observed, as such collisions generate two problems: plastic energy dissipation and energy dissipation by damping.

The dissipation of plastic energy comes from shocks with plastic deformations, representing a small portion of the problems, as seen in Figure 9, as the grains have high resistance (configured parameter) [6,21]. The energy dissipation by damping, which undoubtedly represents the largest portion of energy at the end of the simulation, comes from the energy dissipation linked to the collision between the grains (heat loss, energy absorption by the structure), demonstrating the importance of this parameter for the simulations, considering real applications [9,12,18].

It is also noted that throughout the process the elastic potential energy remains constant, as the configuration of the grains means that

```
# -*- coding: utf-8 -*-

from yade import pack, plot
import time
import random
import math
from yade import ymport

utils.readParamsFromTable(descriptionIn = 'noDescription',
  frIn = 0.5, enIn=0.01, etIn=0.01, tcIn=0.0001,
  rhoIn = 1500.0,
  dumpVTKIn = 4000
)

from yade.params.table import *

import shutil

try:
  shutil.rmtree('cpt')
except OSError:
  pass
os.mkdir('cpt')

altura = 0
rMed = 0
angRepouso = 0
contParticulas = 0

mat1 = O.materials.append(ViscElMat(frictionAngle=frIn, density=rhoIn,tc=tcIn, en=enIn, et=etIn,))
O.bodies.append(ymport.gmsh("hourglass.mesh",scale=500, color=(1,0,1),mask=5))
O.bodies.append(geom.facetBox((0, 0, -8), (10, 10, 0), wallMask=63, color=(1,1,1), wire=False))

sp=pack.SpherePack()
sp.toSimulation()
sp.makeCloud((-3, -3, 5), (3, 3, 8), rMean=.2, rRelFuzz=.3)
sp.toSimulation(color=(.9, .9, .8))
```

Figure 1: Code for simulating grain flow in a silo – YADE (1).

```
for b in O.bodies:
        if not isinstance(b.shape,Sphere): continue
        contParticulas=contParticulas+1

O.engines=[
        ForceResetter(),
        InsertionSortCollider([Bo1_Sphere_Aabb(),Bo1_Facet_Aabb()]),
        InteractionLoop(
                [Ig2_Sphere_Sphere_ScGeom(),Ig2_Facet_Sphere_ScGeom()],
                [Ip2_FrictMat_FrictMat_FrictPhys()],
                [Law2_ScGeom_FrictPhys_CundallStrack()]
        ),
        NewtonIntegrator(gravity=(0,0,-9.81),damping=.75),
        PyRunner(command='checkUnbalanced()',realPeriod=2),
        PyRunner(command='addPlotData()',iterPeriod=100)
]

O.dt=1*PWaveTimeStep()

O.trackEnergy=True
```

Figure 2: Code for simulating grain flow in a silo – YADE (2).

```
def checkUnbalanced():
        if unbalancedForce()<.01:
                O.pause()
                plot.saveDataTxt('bbb.txt.bz2')
                for b in O.bodies:
                        if not isinstance(b.shape,Sphere): continue
                        '''if b.speed > vMax:
                                b.speed = vMax'''

                        print(round(b.state.refPos[0], 2), round(b.state.refPos[1], 2), round(b.state.refPos[2], 2))

                        if round(b.state.refPos[2], 2)>altura:
                                altura = round(b.state.refPos[2], 2)
                        rMed += sqrt(round(b.state.refPos[0], 2)**2 + round(b.state.refPos[1], 2)**2)

                rMed /= contParticulas
                angRepouso = math.atan(altura/rMed)

                print('')
                print('Pilha com ' + str(contParticulas) + ' particulas')
                print('Altura da pilha: ' + str(round(altura, 2)))
                print('Raio medio da pilha: ' +  str(round(rMed, 2)))
                print('Angulo de repouso da pilha: ' + str(round(angRepouso, 2)))

def addPlotData():
        plot.addData(i=O.iter,unbalanced=unbalancedForce(),**O.energy)

plot.plots={'i':('unbalanced',None,O.energy.keys)}
yade.plot.live = True
yade.plot.autozoom = True

plot.plot()

O.saveTmp()

yade.plot.saveDataTxt("teste.txt", vars=O.time)

from yade import qt
qt.View()
r=qt.Renderer()
```

Figure 3: Code for simulating grain flow in a silo – YADE (3).

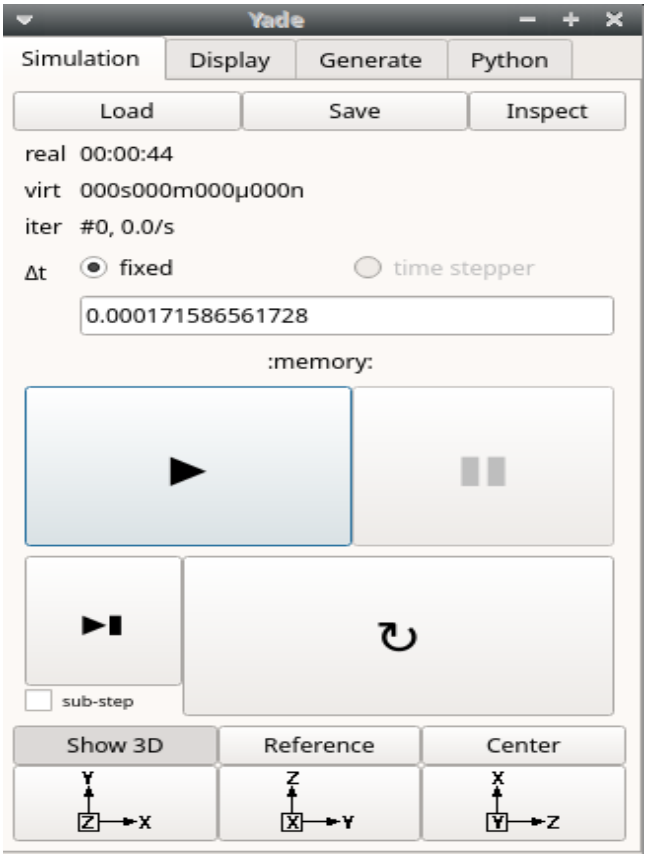

Figure 4: YADE Command Window.

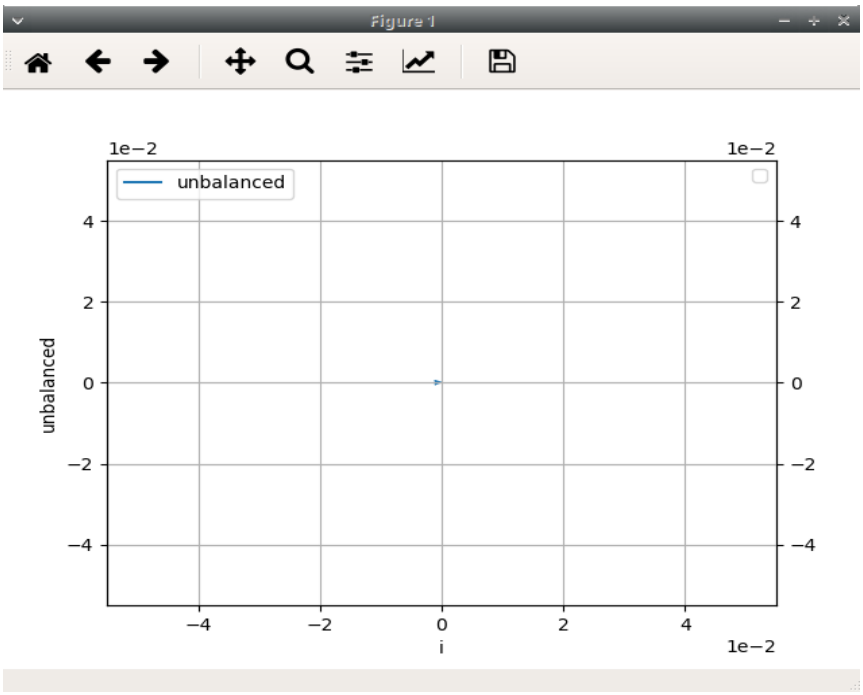

Figure 5: Graph of internal system energies.

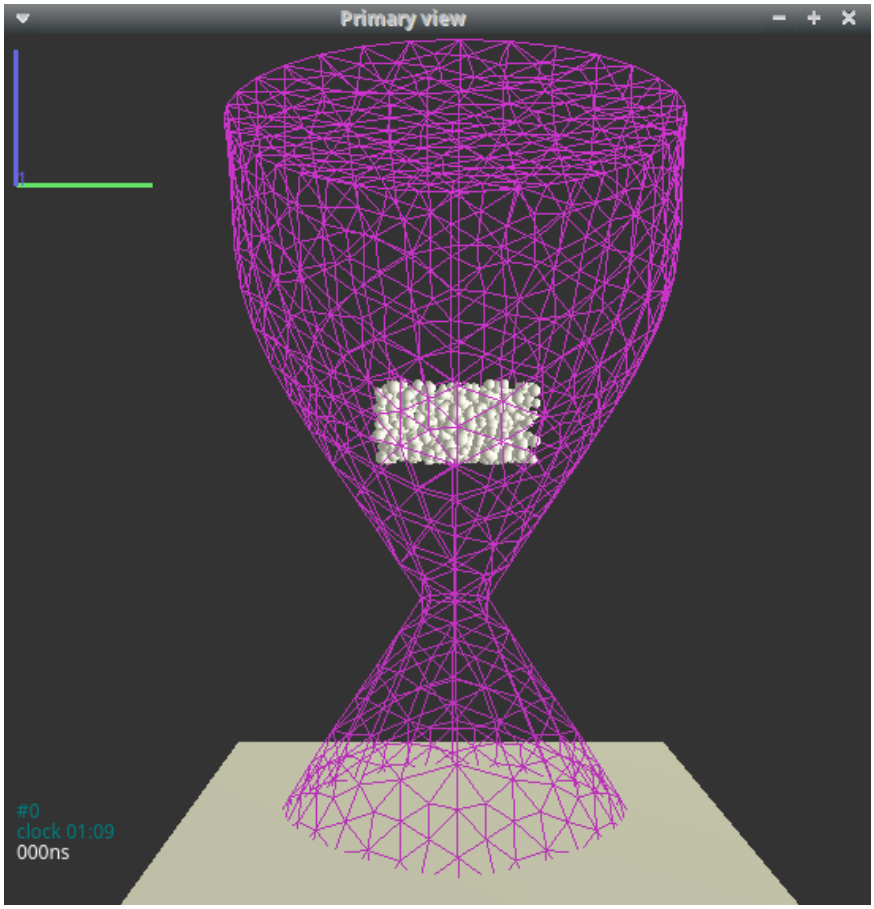

Figure 6: Visual representation of the grains flowing in the silo (initial moment).

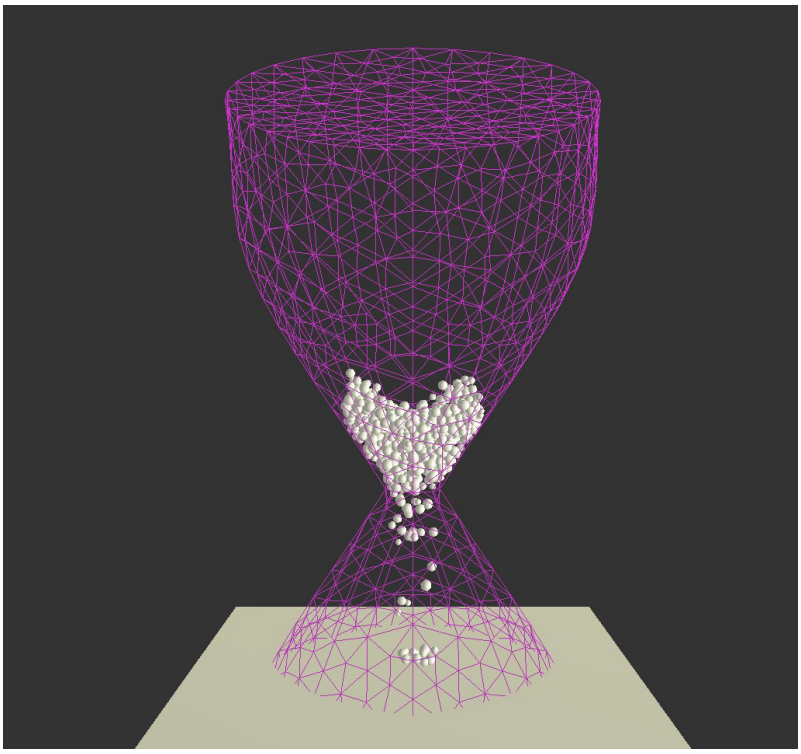

Figure 7: Beginning of the falling grain movement in collision with the silo walls.

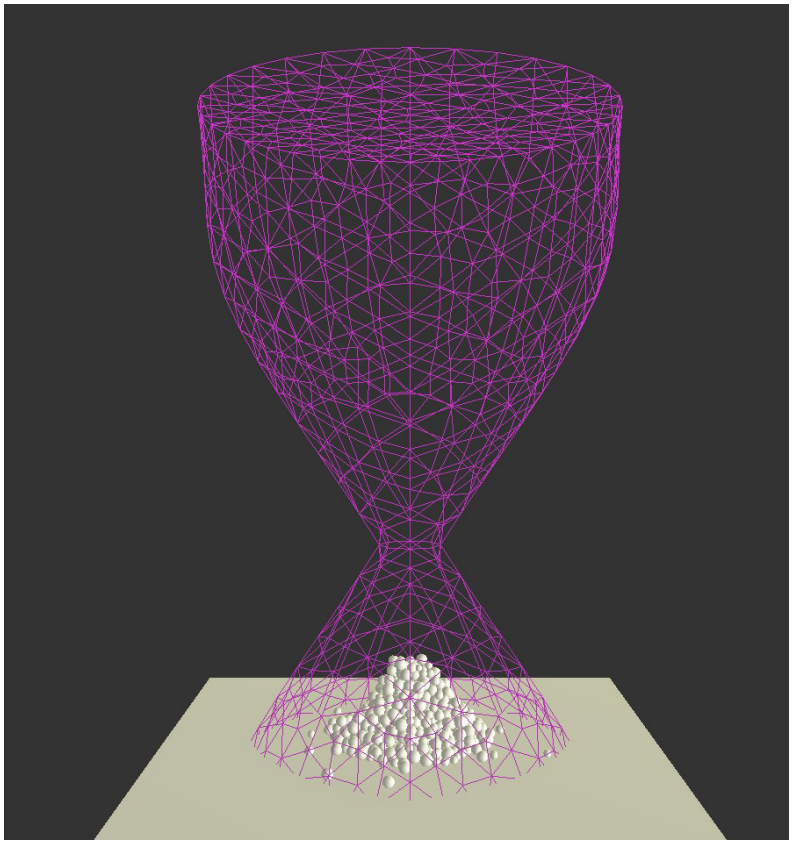

Figure 8: pile formed after the flow of grains through the silo hole.

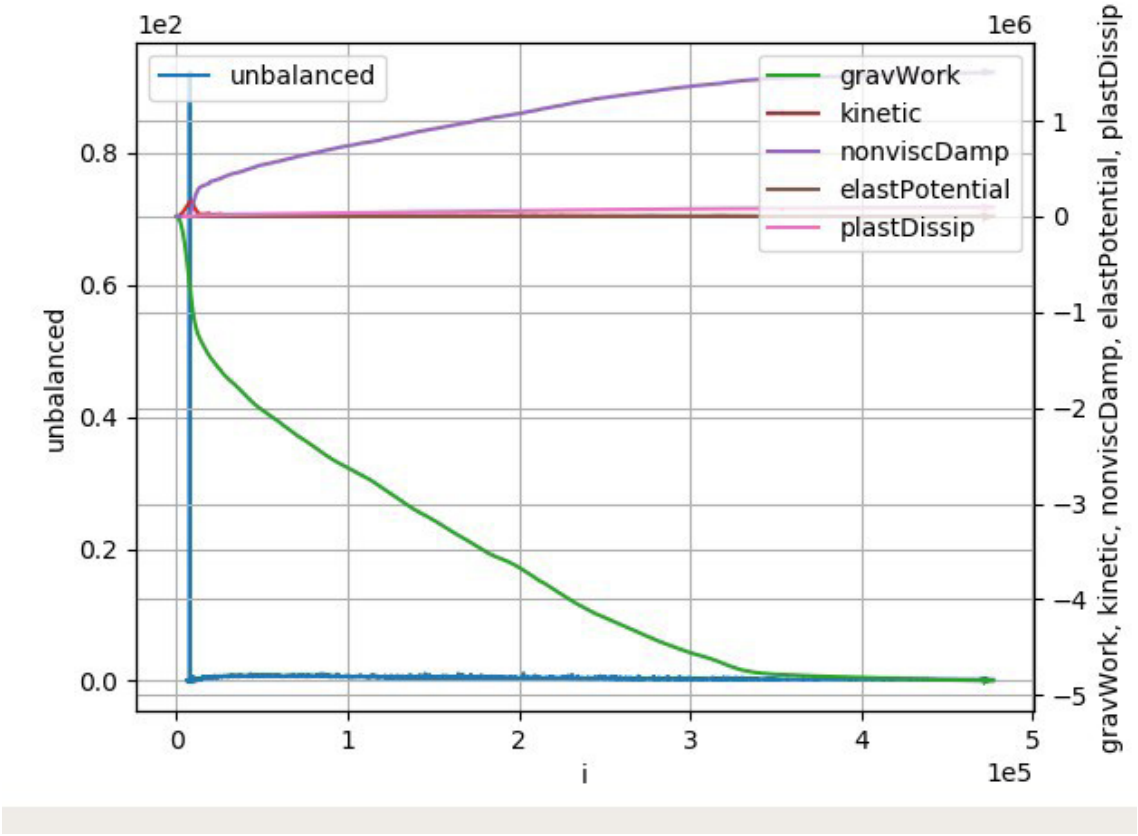

Figure 9: Graph with energy demonstration after running the simulation.

they do not deform to the point of being able to return any energy to the system.

Now the key point of this simulation is to understand what unbalanced energy is all about, and why it is used as a stopping criterion for the simulation, as noted in the code. The unbalanced energy, in fact, is a compensation of energies of a system made by simulation [3,8]. This is due to the conservation of total energy in a closed system, in which energy only changes but is always conserved. But in the computational world there is something important to be taken into account, the truncation [8,13,21].

Truncation is nothing more than the inability of a computer to load all the information from a real system [3,4]. Far from it, the computer actually tends to have its limit of decimal places quite short, when compared to a real system. Therefore, rounding errors regarding the real position of the particles, edges for their collision, approximate speeds, among other variables, make the sum of the internal energies of the system not remain constant and oscillate [21]. Hence the need for unbalanced energy.

Still on figure 9, the unbalanced energy curve (blue) shows a greater oscillation at the initial instant of the simulation. This can be explained by the generation of the particles themselves and their attachment in the simulation, however, it decreases over time, tending to zero at a final instant [1,5,6]. When this energy reaches a sufficiently small value (depends on the accuracy of the simulation), it indicates that this simulation has achieved its purpose, that is, the parameters are close to the real ones. Thus, justifying this parameter to be the stopping criterion of the simulation.

Finally, the last analysis to be performed is the return of the final results. After executing the problem, we will have three values to be analyzed: Final stack height, average stack radius and stack repose angle. This is generated after running the code, shown in Figure 10.

```
Pilha com 1714 particulas
Altura da pilha: 1.04
Raio medio da pilha: 0.56
Angulo de repouso da pilha: 30.87
```

Figure 10: values of the final parameters of the grain pile after running the simulation.

Based on these parameters, operators will be able to make decisions regarding the alteration of some process parameter.

CONCLUSIONS

The implementation of the code performed by the YADE software was successful. This is worth mentioning, as this software uses the Python language and is freely accessible.

The compiled code has the possibility to vary the grain flow and in different geometries, visualizing the results of these parameter variations and also their graphic simulation. In addition, the code makes it possible to visualize the energies involved in the system, thus being able to carry out a careful evaluation of the process.

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