Trajectory of Particle Motion by Particle – Particle Contact Using Discrete Element Method

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Abstract

The objective of this contribution is to exist a numerical simulation technique to model the collision of particles in a plane using object-oriented procedures. This approach is based on the second law of Newton for the translational motion of each particle in the granular material. This comprises a possession track of all forces acting on each particle at every time-step. The back-ground version of DEM and time integration algorithm are established and executed into C++ code. A simple test is regarding the application of time-integration algorithm by particle-particle interaction for which analytical expression exist. In this paper effect of elastic, elastic damping and elastic damping gravitational effect are studied and the trajectory of particle motion for different time integration scheme verses time step for particle – particle contact are calculated.

Keywords — *DEM simulation, Granular materials, Elastic effect, damping effect, trajectory;*

I. INTRODUCTION

A granular material is a conglomeration of many discrete solid particles which is characterized by a loss of energy due to dissipative collisions whenever the particles interact. They can be considered as the fourth state of matter which is very different from solids, liquids or gas. Granular materials are very simple. If the particles are non-cohesive, then the forces between them are basically only repulsive so that the shape of the material is determined by external boundaries and gravity. Practically many solid particles which we make use of in the kitchen are granular particles like sugar, rice, coffee, cereals etc. Walking outside we step on the soil which is again a particulate and hence falls under the category of granular matter. The unusual and unique character displayed by granular material systems have led to a resurgence of interest within several scientific and engineering disciplines ranging from physics, soil mechanics and chemical engineering (Jaeger and Nagel [1992]; Behringer [1995]; Bideau and Hansen [1993]; Jaeger et al. [1994, 1996a]). Much of the engineering literature has been dedicated to understanding how to deal with these materials. Prominent contributions in the literature include Coulomb [1773], who proposed the ideas of static friction; Faraday [1831], who discovered the convective instability in a vibrated container filled with powder, and Reynolds [1885], who introduced the motion of dilatancy, which implies that a compacted granular material must expand in order for it to undergo shear. Processes involving particulate or granular flows are prevalent throughout the pharmaceutical, chemical, energy, food handling, mineral processing, powder metallurgy, and mining industries. In addition, numerous phenomena found in nature involve such material flows.

The discrete element method (DEM), originally developed by Cundall and Strack [1971, 1979], has been used successfully to simulate chute flow (Dippel et.al 1996), heap formation (Luding, 1997), hopper discharge (Thompson and Grest, 1991; Ristow and Herrmann, 1994), blender segregation (Wightman et al., 1998; Shinbrot et al., 1999; Moakher et al., 2000) and flows in rotating drums (Ristow, 1996; Wightman et al., 1998). The DEM allows for the simulation of particle motion and interaction between the particles. DEM considering not only the obvious geometric and material effects such as particle shape, material non-linearity, viscosity, friction, etc., but also the effect of various physical fields of surrounding media, level of chemical reactions (Kantor et al. 2000). One of the most auspicious area of future applications of discrete element method seems to be geotechnical engineering. The discrete approach assumes the soil is an assembly of granular or discrete particle.

II. DISCRETE STATE FORMULATION.

The dynamic behavior of granular media is considered as the dynamics of each particles. The overall response of media is foretold by the behaviour of individual particles and the dynamics of particles is evaluated by applying the second Newton's law. Detection of interaction force between contacting particles is considered by discrete approach is one of the most important issues. The interaction forces of each contacting particle are locally resolved based on actual geometry of kinematic contact between two spherical particles, inter-particle contact forces and boundary conditions.

Granular material is considered as a collection of frictional elastic spherical particles and it is termed as discrete elements. The particles are assumed to be composed of spherical particles with same radii Ri. The granular particles are assumed to be deformable bodies, deforming each other by normal and shear force. The composition of media is time-dependent because distinct particle changes their position by free rigid body motion or by contacting with neighbour particles or walls. Each particle may be in contact with other particles. The boundary conditions of media are determined by planes and treated as particles with an infinite radius and mass

III.GEOMETRY OF KINEMATIC CONTACT OF SPHERICAL PARTICLES

Consider two particles i and j be in contact with position vectors x_i and x_j with center of gravity lying at O_i and O_j having linear velocities v_i and v_j .

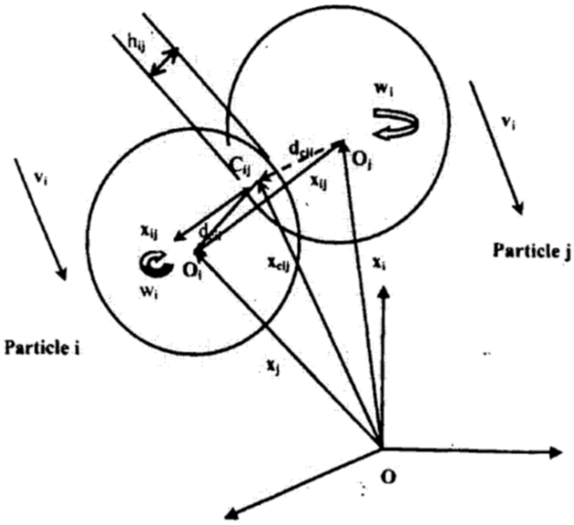

Figure 1. Inter particle Contact between two identical spheres *i* and *j*

The contact point C_{ij} is defined to be at the center of the overlap area position vector x_{cij}.The vector x_{ij} of the relative position point from the center to gravity of particle i *to* that of particle j is defined as $x_{ij} = x_i - x_j$ The depth of overlap ish_{ij}. Unit vector in the normal direction of the contact surface through the center of the overlap area is denoted by n_{ij}. It extends from the contact point to the inside of the particle i as $n_{ij} = -n_{ji}$

Since the particle shape is assumed to be spherical, for sphere of any dimension the contact parameters can be written as follows:

$$h_{ij} = \begin{cases} R_i + R_j - |x_{ij}|, |x_{ij}| < R_i + R_j \\ 0, |x_{ij}| \geq R_i + R_j \end{cases}$$

Where R_i is the radius of the particle. The relative velocity of the contact point is defined as

$$v_{ij} = v_{cij} - v_{cji}$$

IV.INTER PARTICLE CONTACT FORCE

The contact force between particles can be expressed as the sum of normal and tangential components;

$$F_{ij} = F_{n,ij} + F_{t,ij}$$

The contact forces between particles depend on the overlap geometry, the properties of the material and the relative velocity between the particles in the contact area and it is modeled as spring, dash-pots and a friction slider. If the particles are in perfect contact model, it is required to describe the effects of elasticity, energy loss through internal friction and attraction on the contact surface for the contact force calculations. The normal component of contact force between particles can be expressed as the sum of elastic force and viscous force.

$$F_{n,ij} = F_{n,ij,elastic} + F_{n,ij,viscous}$$

Normal elastic force is based on the linear Hooke's law of a spring with a spring stiffness constant $k_{n.ij}$ and is given by the expression,

$$F_{n,ij,elastic} = K_{n,ij} h_{ij} n_{ij}$$

Normal viscous force is dissipated during real collisions between particles. The linear dependency of force on the relative velocity of the particles at the contact point with a constant normal dissipation coefficient γ_n and is expressed as

$$F_{n,ij,viscous} = -\gamma_n m_{ij} v_{n,ij}$$

Equation for the motion of granular material in a plane,

$$m_i \frac{d^2 x_i}{dt^2} = m_i a_i$$

$$= F_i$$

$$v_i = \frac{dx_i}{dt}$$

Force acting on i^{th} particle F_i is, $F_i = m_i g + \sum_{\substack{j=i \\ j \neq i}}^{N} F_{n,ij} + \sum_{\substack{j=i \\ j \neq i}}^{N} F_{t,ij}$ *i.e.*, sum of gravitational force and contact force

V. COMPUTER IMPLEMENTATION

The key computational tasks of DEM at each time step of contact particle can be summarized as follows*:*

- Finding of contacts between a particle *i* and *j*.
- Calculation of contact forces from relative displacement between particles
- Summary of contact forces to determine the total unbalanced force
- Computation of acceleration from force
- Velocity and displacement by integrating the acceleration
- Updating the position of particles

VI. RESULT AND DISCUSSION

A. Particle – Particle Contact by Discrete Element Method

The evaluation of the time integration scheme depends on calculation time resource presenting the most important part of the numerical simulation technique of DEM. The time integrating scheme with different time steps were examined. Here several model of normal contact forces are considered:

1. Normal elastic force;
2. Normal elastic and damping forces;
3. Normal elastic, damping and gravity forces;

The normal force is composed of linear spring force and a dashpot force where spring produces an elastic repulsive force and the dashpot contributes to the damping and is mathematically expressed as

$$F_n = m_{ij}\ddot{\delta} + C_n\dot{\delta} + K_n\delta$$

Where δ is the overlap depth between the contacting pairs, $m_{ij}, K_n \; and \; C_n$ are the reduced mass the normal spring stiffness and normal damping (dissipation) coefficients, respectively. The first derivative of the overlap $(\dot{\delta})$ corresponds to the relative normal velocity in physical sense. Subsequently, the second derivative of the overlap $(\ddot{\delta})$ corresponds to the relative normal acceleration. To test the particle-Particle collision the first particle moving at the initial velocity and hitting the second particle. In these tangential forces are set to be zero. Various integration schemes for numerical solution of differential equation can be used, but 5th order Gear predictor-corrector scheme (Alien and Tildseley, [1987]) is used in this work to solve the equations, which is stable for second-order differential equations.

1) Normal Elastic Force

For this test, parameters corresponding to the tangential and damping forces are set to be zero and the elastic effect alone is studied. This test also confirms the particle-particle interaction. Here the trajectory of particle motion for different time integration schemes verses the time step and the collision time are calculated using discrete element method. Here the time steps are considered as 0.0005, 0.0001 seconds.

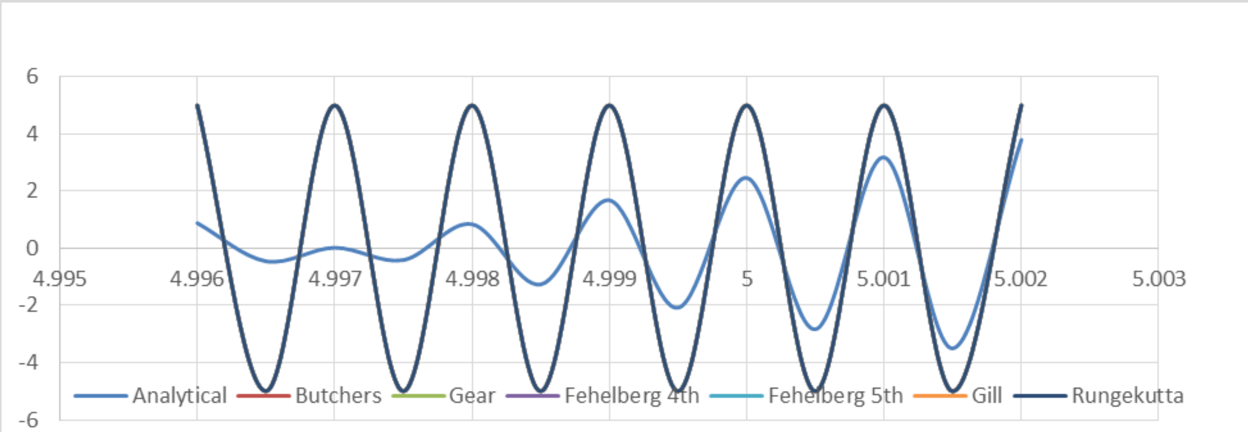

Figure 1. The elastic effect for the trajectory of particle motion for different time integration scheme verses time step0.005

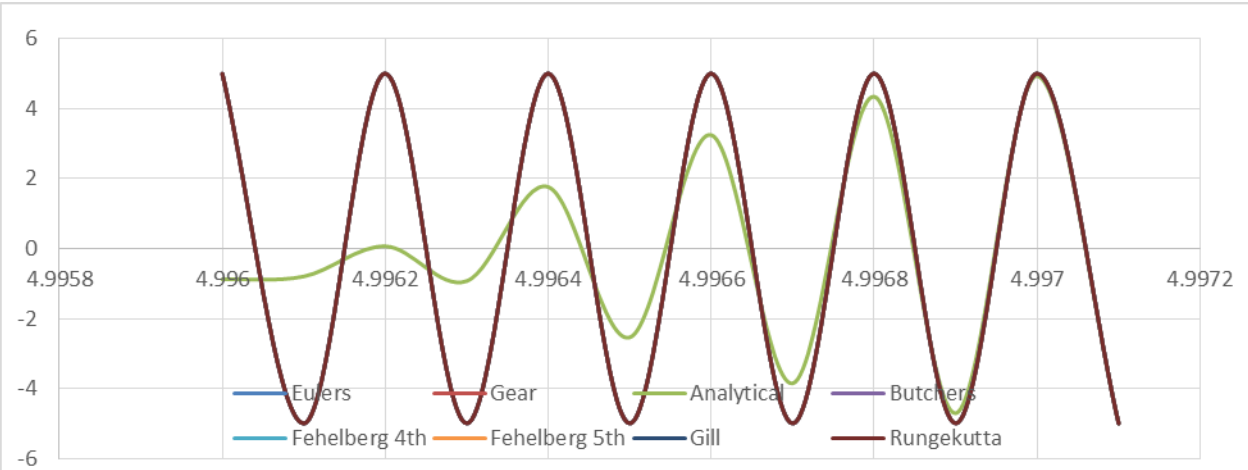

Figure 2. The elastic effect for the trajectory of particle motion for different time integration scheme verses time step 0.0001

DEM in which a large time step is possible in developed by improving the algorithm to solve the contact forces between two particles. Here fourth order Runge-Kutta method, Rungekutta Gill, Rungekutta Fehelberg 4th order, Rungekutta Fehelberg 5th order, Runge- kutta Butcher's fifth order and Gear Predictor-Corrector method are applied to solve second order initial value problem (IVP) of ordinary differential equation (ODE). We can find that the same value is obtained by fourth order Runge-Kutta method, Rungekutta Gill, Rungekutta Fehelberg 4th order, Rungekutta Fehelberg 5th order, Runge- kutta Butcher's fifth order. By comparing the result with analytical method we can find that Gear predictor corrector method is more accurate than other methods. To find more accurate results we increase the step size. From the figure.1 and figure2 we can see that both methods give almost same results but Gear Predictor-Corrector method gives more accurate than other methods.

*2) **Normal elastic, damping force***

For this test, parameters corresponding to the tangential and gravitational forces are set to be zero and the elastic, damping effect is studied. This test also confirms the identical particle by particle-particle interaction. Here the trajectory of particle motion for different time integration schemes verses the time step and the collision time are calculated.

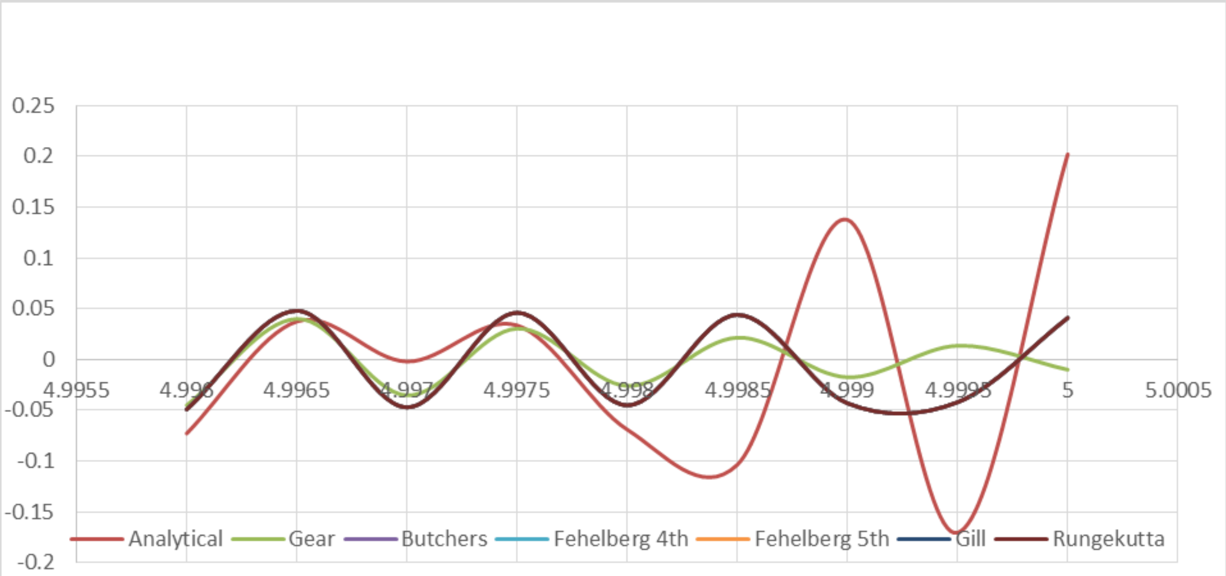

Figure 3. The elastic damping effect for the trajectory of particle motion for different time integration scheme verses time step 0.0005

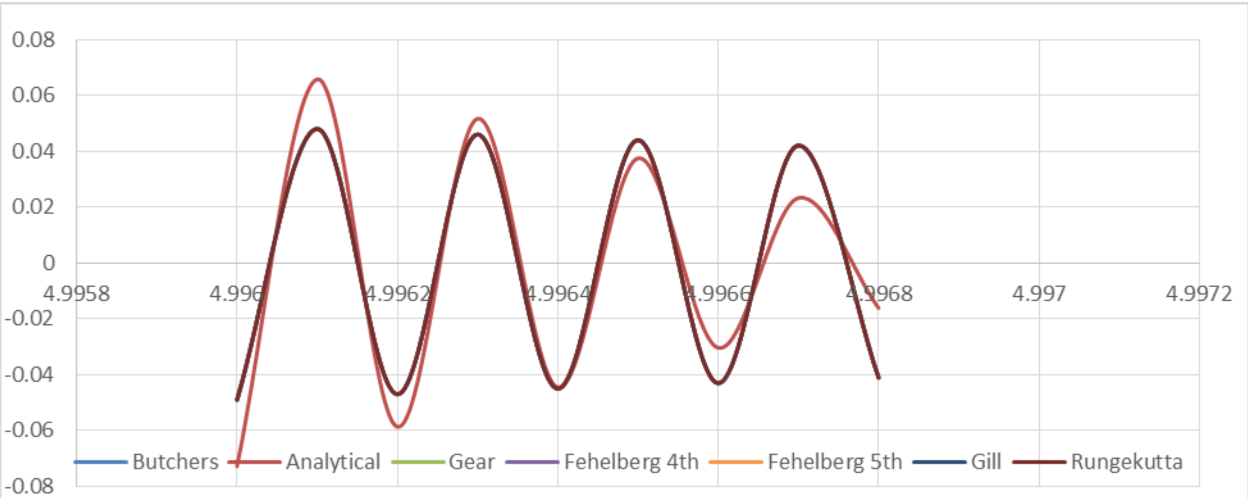

Figure 4. The elastic damping effect for the trajectory of particle motion for different time integration scheme verses time step 0.0001

When time step increases we get more accurate value. Time of collision is greater in 0.0001 compared with 0.0005 seconds. From the figure.3 and figure 4 we can see that both methods give almost same results but Gear Predictor-Corrector method gives more accurate results than fourth order Runge-Kutta method, Rungekutta Gill, Rungekutta Fehelberg 4^{th} order, Rungekutta Fehelberg 5^{th} order, Runge- kutta Butcher's fifth order. By comparing trajectory of particles in collision for elastic effect and elastic damping effect, we can see more collision is occurred in elastic effect than elastic damping effect. More displacement is occurred in damping effect than elastic effect.

3) Effect of elastic, damping and gravitational force

For this test, parameters corresponding to the tangential force are set to be zero and the elastic, damping and gravitational effect is studied. This test also confirms the identical particle by particle-particle interaction. Here the trajectory of particle motion for different time integration schemes verses the time step and the collision time are calculated.

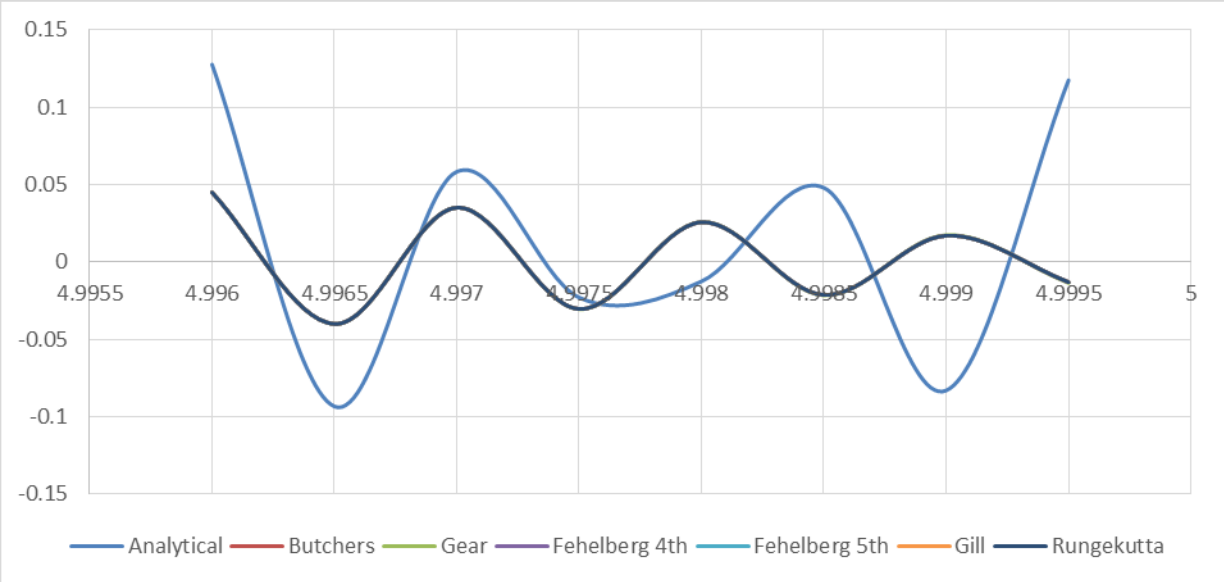

Figure 5. The elastic damping gravitational effect for the trajectory of particle motion for different time integration scheme verses time step 0.0005

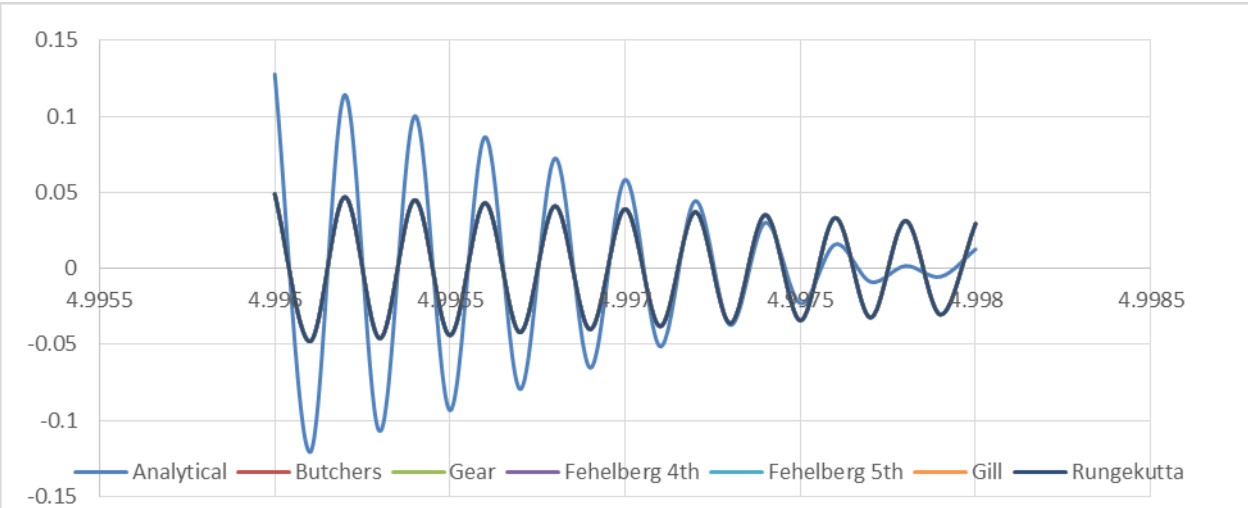

Figure 6. The elastic damping gravitational effect for the trajectory of particle motion for different time integration scheme verses time step 0.0001

From the result we can find that time step increases we get more accurate value. Time of collision is greater in 0.0001 compared with 0.0005 seconds. From the figure.5 and figure 6 we can see that both methods give almost same results but Gear Predictor-Corrector method gives more accurate results than fourth order Runge-Kutta method, Rungekutta Gill, Rungekutta Fehelberg 4^{th} order, Rungekutta Fehelberg 5^{th} order, Runge-kutta Butcher's fifth order. By comparing elastic, elastic damping and elastic damping gravity effect we get more collision in elastic damping gravitational effect than the other two effect. Least collision is occurred in elastic effect. By comparing the three effects elastic damping effect acquire more displacement than the other two effects.

VII.CONCLUSION

The result obtained in the present investigation may be generally described as follows:

- The described discrete element model composed of visco-elastic spherical particles is implemented into the developed C++ code. The analytical solutions for the impact of two spheres have been examined and derived.

- By comparing elastic, elastic damping and elastic damping gravity effect we get more collision in elastic damping gravitational effect than the other two effect.
- Least collision is occurred in elastic effect.
- By comparing the three effects elastic damping effect acquire more displacement than the other two effects

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