

Numerical simulations of N-body problems under $1/r^2$ force laws

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An investigation of numerical solutions to a gravitational and an electrostatic classical N-body problem are discussed. Simulations written in Python are presented, which use the ODEint function from the SciPy library to perform numerical integration. Trajectories of a satellite approaching the planet Mars are investigated using plane polar, Cartesian and Jacobi coordinates. Rutherford's and Thomson's models of the atom are compared by a simulation of alpha particle scattering, confirming the result that the atom must consist of a very small positively charged nucleus.

Introduction

In classical physics, Newton's law of gravity and Coulomb's law of electrostatics provide good explanations for phenomena on vastly differing scales, yet both have fundamentally the same mathematical form. They are both force laws which vary as $1/r^2$, where r is the distance between the masses or charges exerting a force on one another. As such, they are both amenable to a similar treatment, and a solution to one problem can easily be transformed into a solution of the other.

In this paper, numerical solutions are presented to a simple gravitational 2-body problem, and a more complicated electrostatic many-body problem. The computational simulations written to solve these problems are explained and the results discussed and compared to those given by an analytic treatment.

In general, numerical methods and efficient computational algorithms are essential in modern physics, as the differential equations describing most real physical systems cannot be solved analytically. This study therefore serves as a simple introduction to the important field of computational modelling.

1 Satellite approaching Mars

Although the classical equations describing the motion of one or two bodies due to a gravitational force can be solved in exact form, the numerical model in this section can be seen as setting a framework that can be extended to multiple astronomical bodies. Such extended simulations are very useful for calculating the motion of rockets, satellites and other man-made and natural bodies. The complicated 'planetary slingshots' undertaken by the Cassini probe on its way from the Earth to Saturn is such an example [1].

The simplicity of the 2-body simulation also allows us to compare it to the exact, closed-form, analytic solution, thus providing insight into the accuracy of the numerical model.

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1.1 The model

To simplify the model of Mars and its satellite, the following approximations were made: Mars was assumed to be a perfect sphere of uniform density and the satellite was taken as being a point mass, since its size is so small compared to that of Mars. This geometry allows the gravitational force on the satellite due to Mars to be treated as identical to that of a point mass located at Mars's geometric centre.

An analytic treatment of a point particle moving under a $1/r^2$ force, shows that four types of trajectory are possible; all being conic sections and lying in a plane. These are: an ellipse, a circle, a parabola and a hyperbola. The particular path traced out depends on the energy of the motion and also on whether the force is attractive or repulsive [2]. For an attractive force, such as gravitation, all four trajectories are possible.

For a satellite approaching an extended body such as a planet, another alternative is that it may collide with the surface. This is really just a case of an elliptic orbit about the planet's centre of gravity, which is a focal point of the ellipse, where the shortest distance from the attempted elliptical path to this focus is smaller than the radius of the planet. The simulation checks for this situation and, should a collision occur, it models the satellite as having coalesced with the planet's surface, coming to an immediate halt.

Various steps of increasing complexity were taken in building up the model. Initially, the motion of the satellite alone was considered as viewed from Mars's frame of reference. The force acting on Mars due to the satellite was ignored, since the far larger mass of Mars means that any change in its motion is tiny compared to that of the satellite. The geometry of this scenario lends itself to an expression in plane polar coordinates (see Appendix A).

After this, the motion of Mars itself was accounted for. Due to its large distance from the sun, the motion of the planet was approximated as being in a straight line. Again forces on the planet were ignored, and only force of Mars on the satellite calculated. Since Mars was now taken as moving in a straight line, Cartesian coordinates provided the simplest expression of the equations of motion (see Appendix B).

Finally, the forces on both bodies were accounted for and the problem expressed in Jacobi coordinates to simplify the mathematics (see Appendix C). Using three different coordinate systems allowed a comparison to be made as to which provided more stable/accurate solutions.

The core simulation logic is outlined in flowchart form in figure 1.

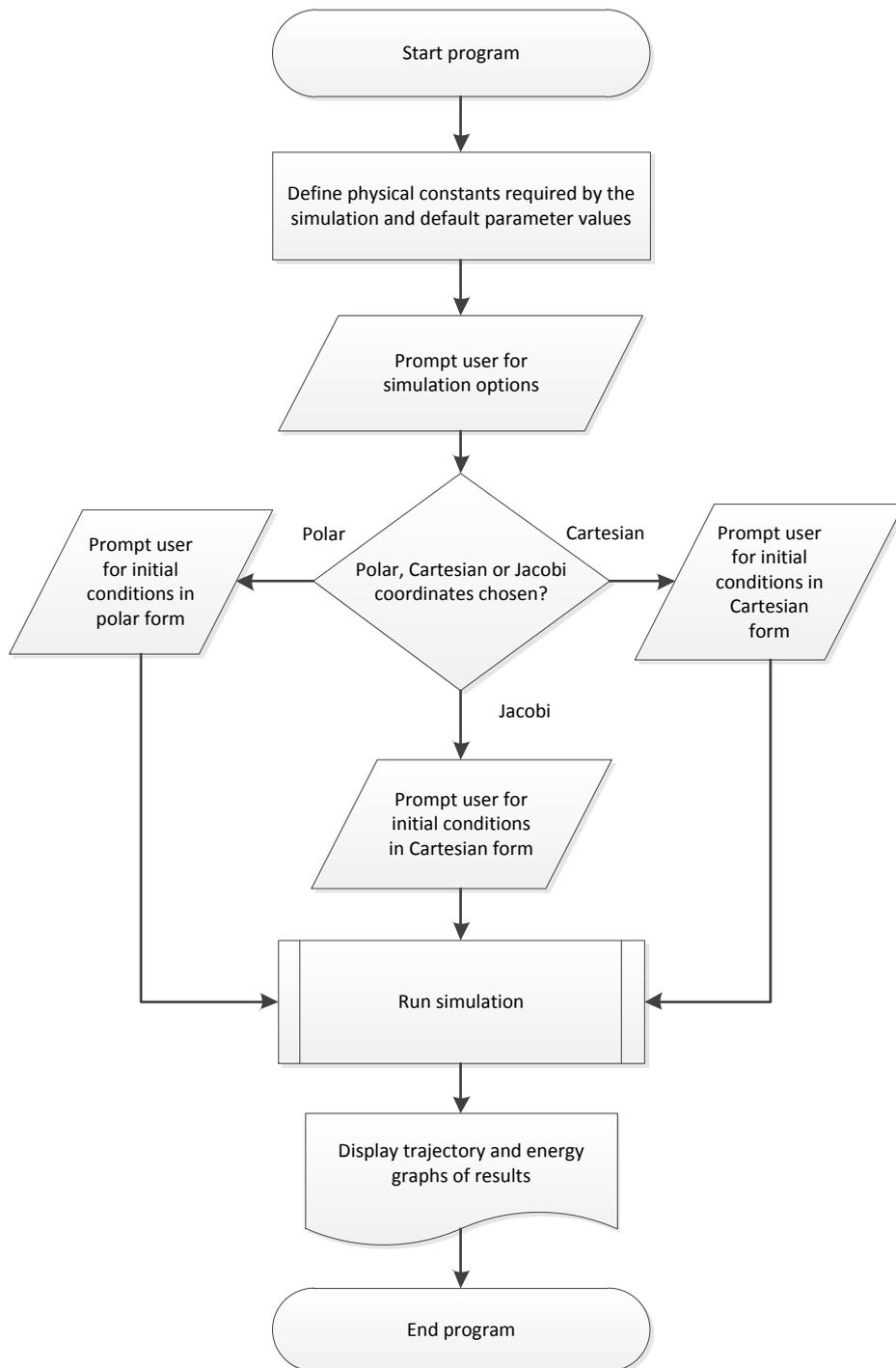


Figure 1:

Flowchart explaining the main application logic for the Mars–satellite simulation. The “Run simulation” sub-process calls the numerical integration routine, ODEint to solve the differential equations over a range of time steps. A separate function is defined for each of the three different coordinate systems, each expressing the system’s equations of motion in terms of derivatives of the state variables (position and velocity).

1.2 Results

The simulation was first used to explore the behaviour of the satellite as it approached Mars in the planet's reference frame. For trajectories where the satellite was not captured into orbit, graphs of its angular deviation were plotted both as a function of impact parameter and of initial velocity. This was achieved via a short section of code temporarily added into the program to loop over the simulation with varying initial conditions. These results matched the theoretical predictions and were thus of limited interest.

However, a more important fact is that in Mars's frame of reference, the satellite's energy should be conserved. Plotting this energy against time shows that the error due to the numerical solution is sensitive both to the form of the differential equations (i.e. the coordinate system used) and to the shape of the trajectory (i.e. the initial conditions). Some example results are shown in figures 2 through 9 below.

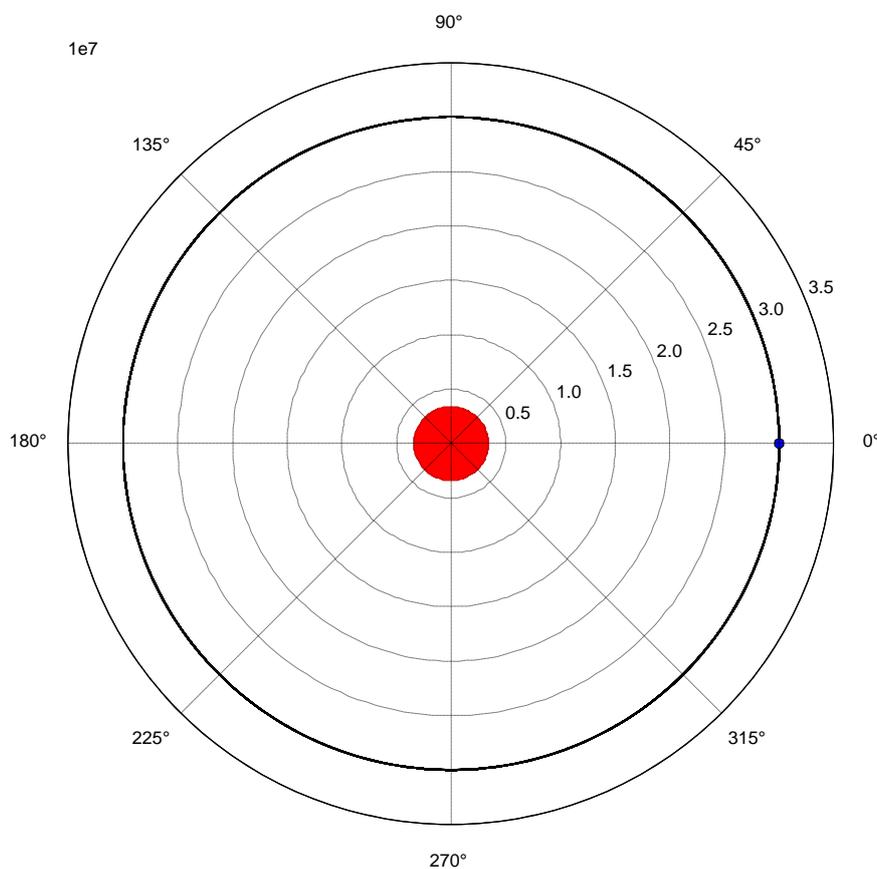


Figure 2:

Circular orbit of satellite around Mars. Initial conditions: $r = 3 \times 10^7$ m, $\theta = 0$, $v_r = 0$ m/s, $v_\theta = 1192.86769314$ m/s. The blue marker illustrates the initial position of the satellite at time $t=0$. Mars is plotted to scale in red. In polar coordinates, energy is found to be conserved extremely well. In Jacobi coordinates, the total energy of Mars and the satellite is also conserved extremely well.

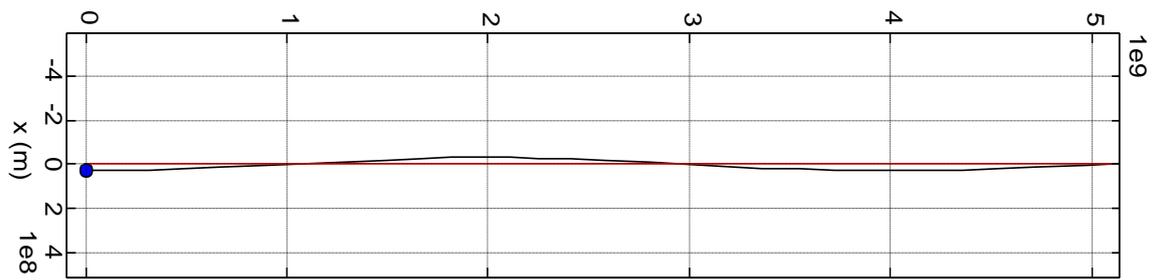


Figure 3:

Motion of satellite around Mars in the same circular orbit, calculated in Jacobi coordinates and viewed in the reference frame of a stationary observer (with respect to the Sun). The locus traced out by the satellite is a contracted cycloid (also referred to as a trochoid).

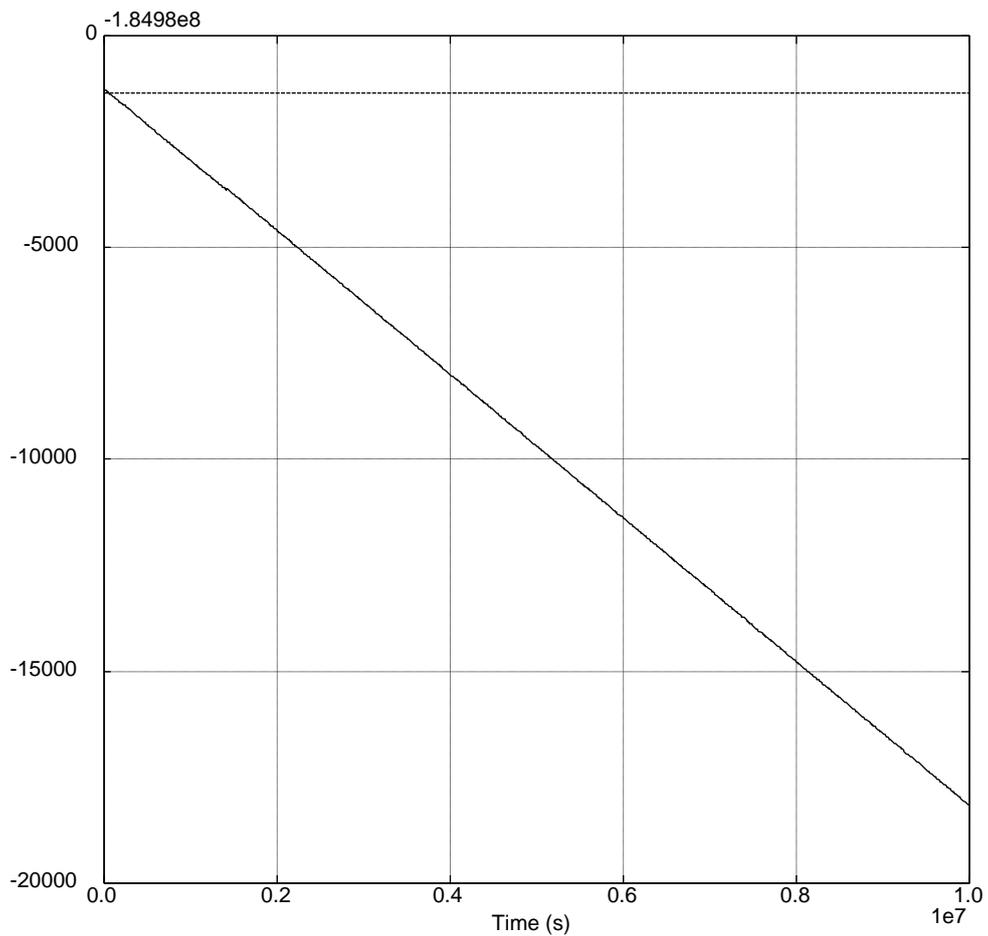


Figure 4: Energy plotted against time for the same circular orbit calculated in Cartesian coordinates. A linear decrease in energy with time is observed from Mars's reference frame. Theoretical value, shown as a dashed line.

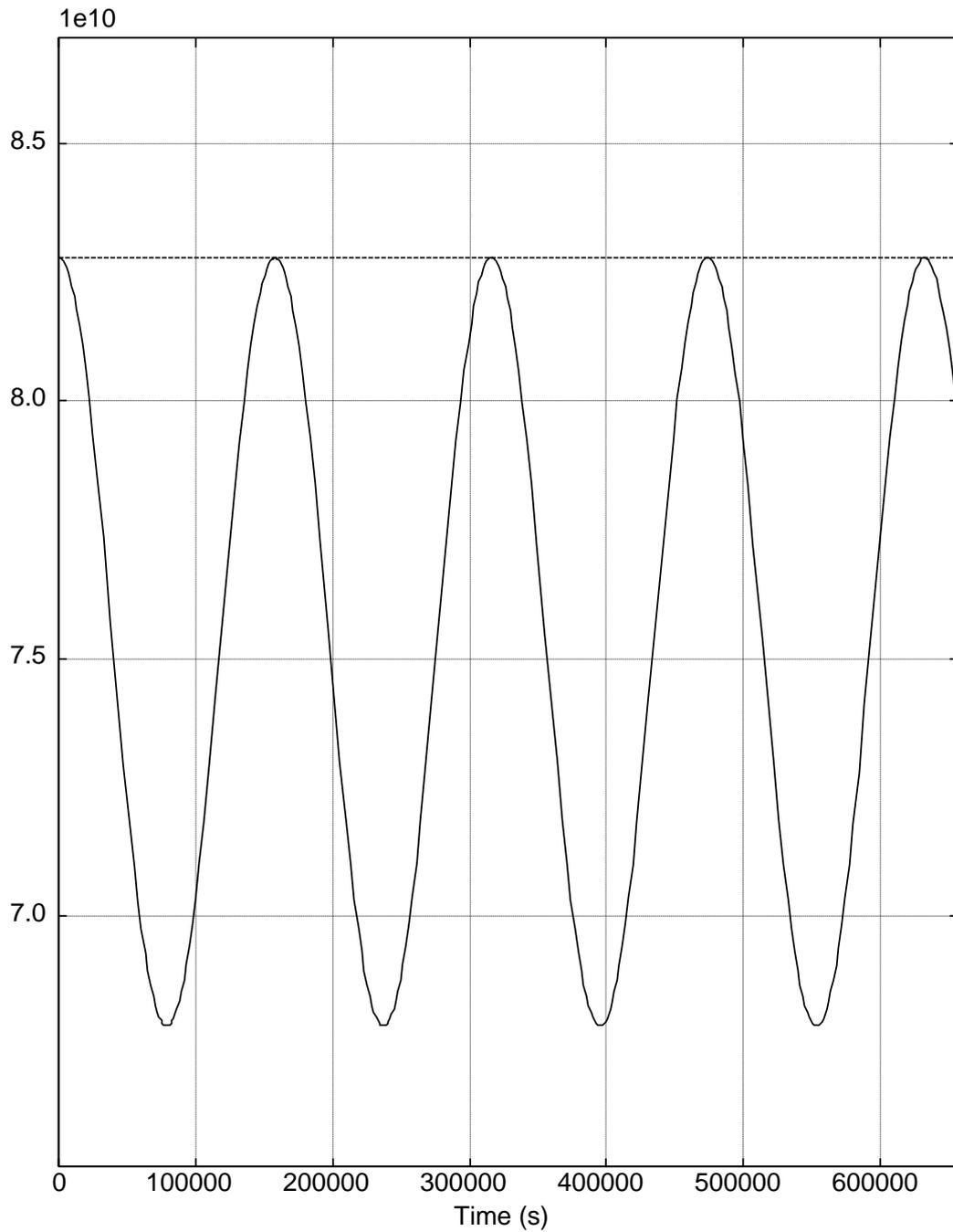


Figure 5:

Energy plotted against time for the same circular orbit calculated in Cartesian coordinates, but this time viewed from a stationary reference frame (with respect to the Sun). The total energy of the satellite oscillates as expected (the energy of the satellite alone is not conserved in this frame of reference since Mars is not stationary), returning periodically to its initial energy (shown as a dashed line).

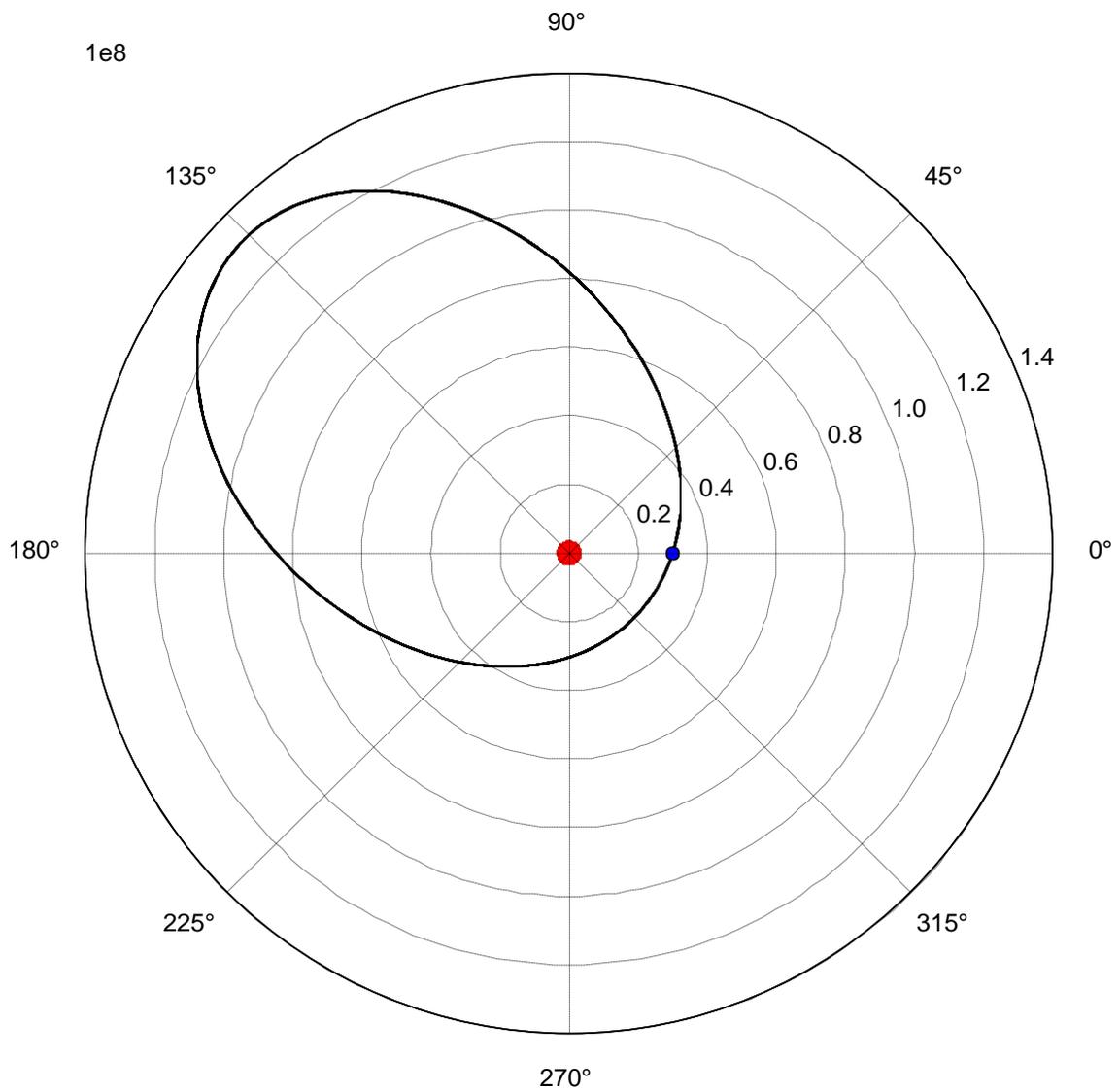


Figure 6:

Trajectory of satellite in an elliptical orbit about Mars. Initial conditions: $r = 3 \times 10^7$ m, $\theta = 0$, $v_r = 450$ m/s, $v_\theta = 1450$ m/s. The blue marker illustrates the initial position of the satellite at time $t = 0$. Mars, plotted (to scale) in red, is at one of the focal points of the ellipse.

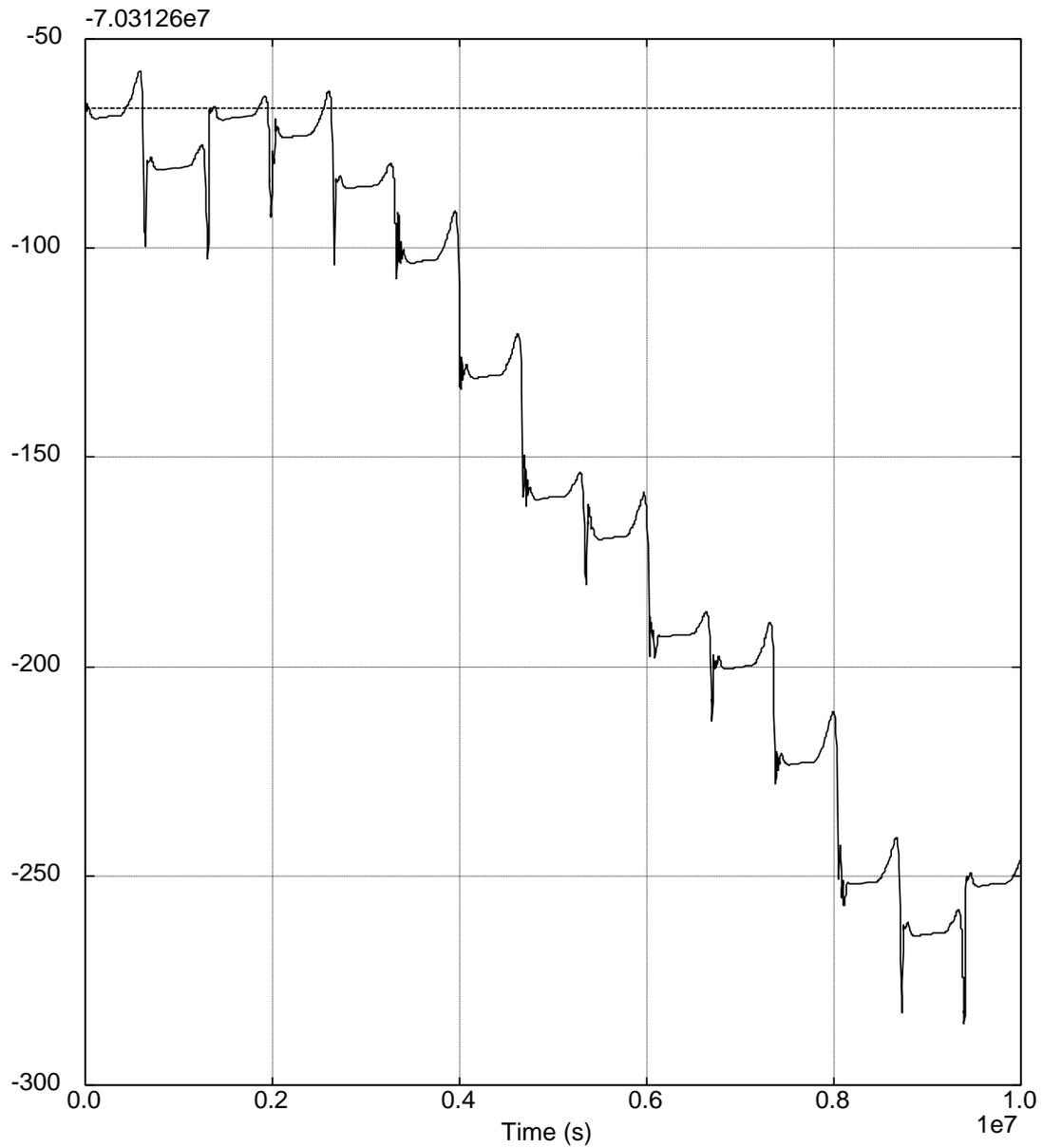


Figure 7:

The satellite's energy when in the same elliptical orbit, as calculated in polar coordinates. The total energy oscillates, but appears to decrease over time. A similar result is found when solving the equations for Mars's frame of reference in Cartesian and Jacobi Cartesian form, although in simple Cartesian coordinates the energy remains closer to its theoretical value (shown as a dashed line) for the first 0.4×10^7 s before dropping.

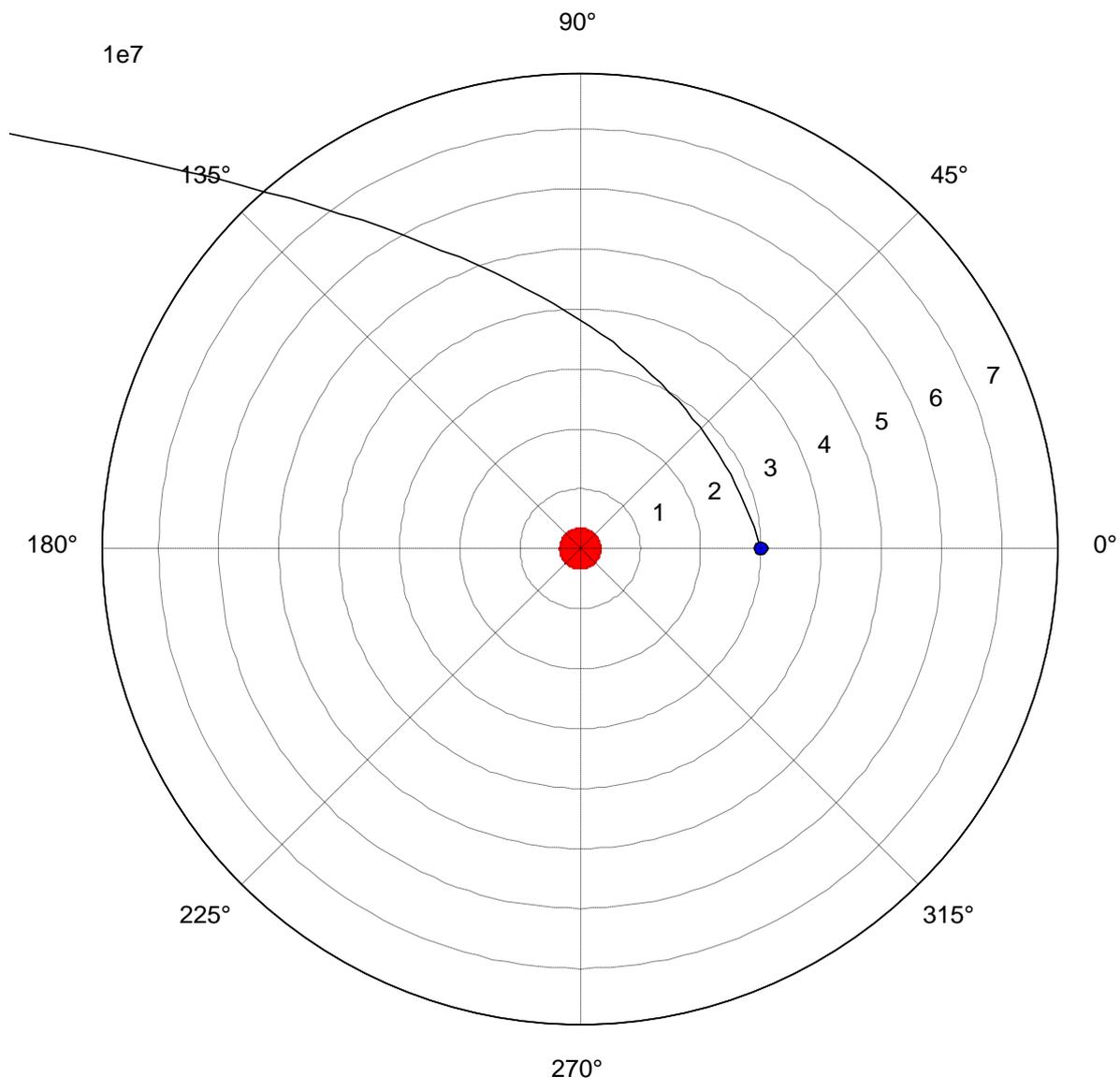


Figure 8:

Hyperbolic trajectory of satellite as viewed from Mars's frame of reference. The initial conditions are: $r = 3 \times 10^7$ m, $\theta = 0$, $v_r = -500$ m/s, $v_\theta = 1700$ m/s. Mars is shown to scale as a red circle at the origin. The blue marker (not to scale) represents the starting point of the satellite at time $t = 0$.

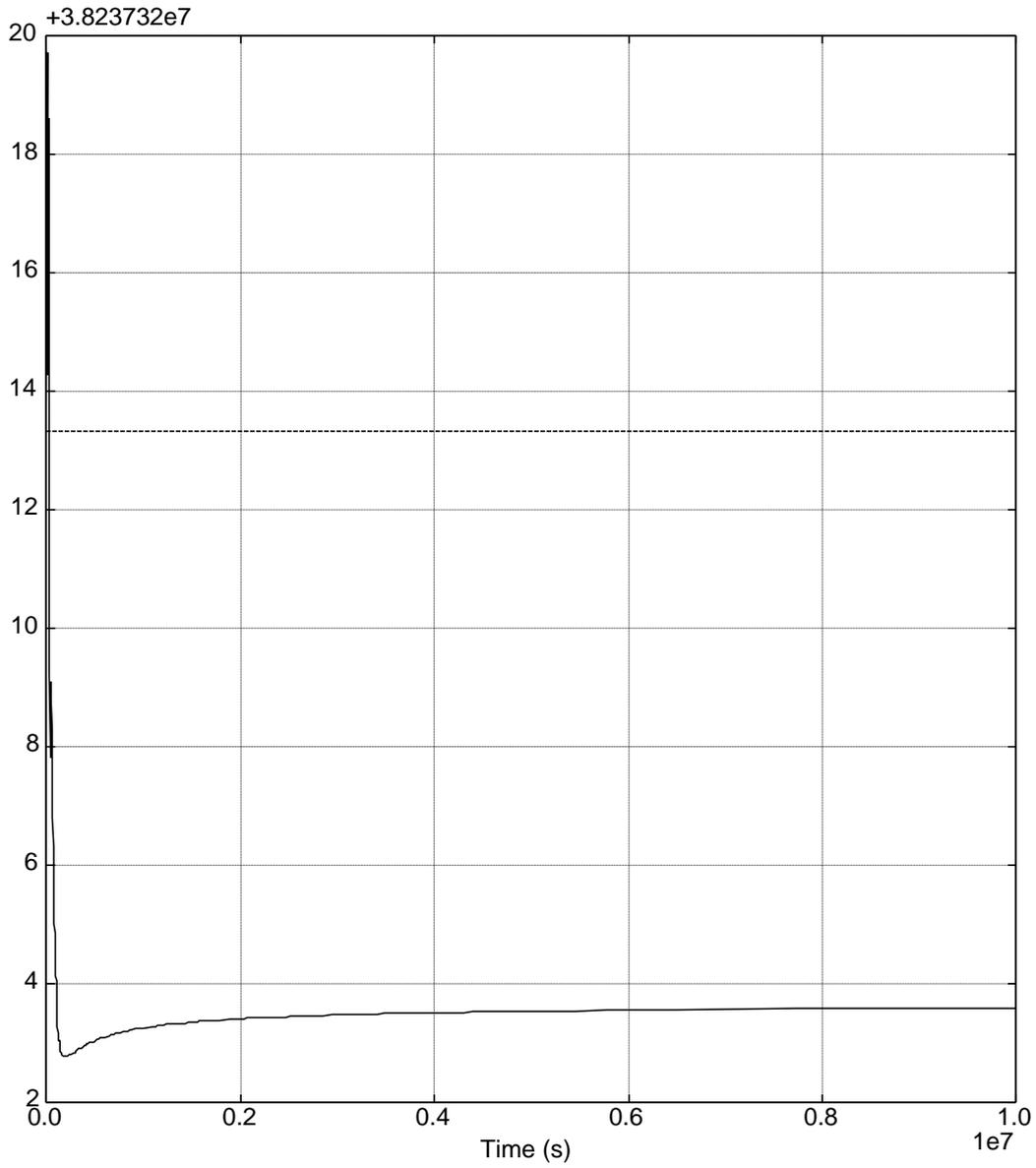


Figure 9:

Satellite's total energy plotted against time for the same hyperbolic trajectory, calculated in polar coordinates. The energy drops suddenly below the theoretical value (shown as a dashed line), but thereafter remains approximately constant. The same behaviour is observed when calculating the energy for the Cartesian or Jacobi solutions in Mars's frame of reference. This latter result is to be expected, since the satellite is effectively performing a reverse 'slingshot' manoeuvre and hence loses some of its energy to Mars. In the frame stationary with respect to the Sun, total energy is found to be conserved when using Jacobi coordinates, as expected. A standard 'gravitational slingshot' can also be demonstrated easily by running the simulation with the appropriate choice of initial conditions.

2 Rutherford scattering

The historical discovery of the atomic nucleus in 1909 by Rutherford, Geiger and Marsden, was due to the now famous alpha scattering experiment, in which a thin gold foil was bombarded by energetic alpha particles [3]. A computer model simulating this experiment was developed, starting from a 2-body system identical in form to that of the Mars– satellite problem discussed above; with the obvious difference that positive alpha particles are repelled by (rather than attracted to) positive charges in the atom.

Prior to Rutherford discovering the nucleus and developing his model of the atom (later to be modified by Bohr), the prevailing model of the atom was that of J. J. Thomson, often referred to descriptively as the “plum pudding” model. This is the idea that the atom is a positive region of charge filling a spherical volume, with negatively charged electrons contained within. Rutherford himself, subscribed to this model before the experiments of Geiger and Marsden showed that this could not possibly describe the physical phenomenon of large angle scattering of alpha particles.

This section describes a simulation that was built to compare the two models computationally and then presents the conclusions drawn from it in support of Rutherford’s work.

2.1 The model

To simplify the simulation, scattering due to electrons was completely neglected. This was for two reasons: first and foremost, any collision between an electron and an alpha particle will cause a negligible deviation to the path of the alpha particle due to its mass being so much larger than that of an electron (4 Atomic Mass Units compared to 0.00055 Atomic Mass Units). In fact, it can be shown that whilst an electron could be scattered by a large angle in such a collision, the alpha particle will always continue in an almost straight path.

Secondly the level of complexity required to model the electrons would be beyond the scope of this work. It is not an insignificant task to consider how and where to model the electrons in an atom. Unlike the stationary nucleus or “pudding” of positive charge, electrons were considered in Classical physics to be undertaking orbits inside the atom. Before his model was ruled out, Thomson himself worked on calculating the possible orbits of electrons in his model of the atom [4].

This simulation thus considers gold atoms as heavy positive ions that are not deflected by the passing alpha particles. They are modelled both as a tiny spherical nucleus (of radius $5 \times 10^{-15} \text{m}$) with nothing but empty space surrounding them, and, contrastingly, as larger spherical regions of positive charge (of radius $135 \times 10^{-12} \text{m}$), through which, however, an alpha particle may travel.

The alpha particles are modelled as approaching the gold foil perpendicularly with an initial kinetic energy of 5 MeV.

For multi atom scattering, the atoms were defined in a rectangular array. In fact gold crystals have a slightly different arrangement, and to further complicate things, there are deviations from this structure in gold leaf due to its thinness causing various strains [5].

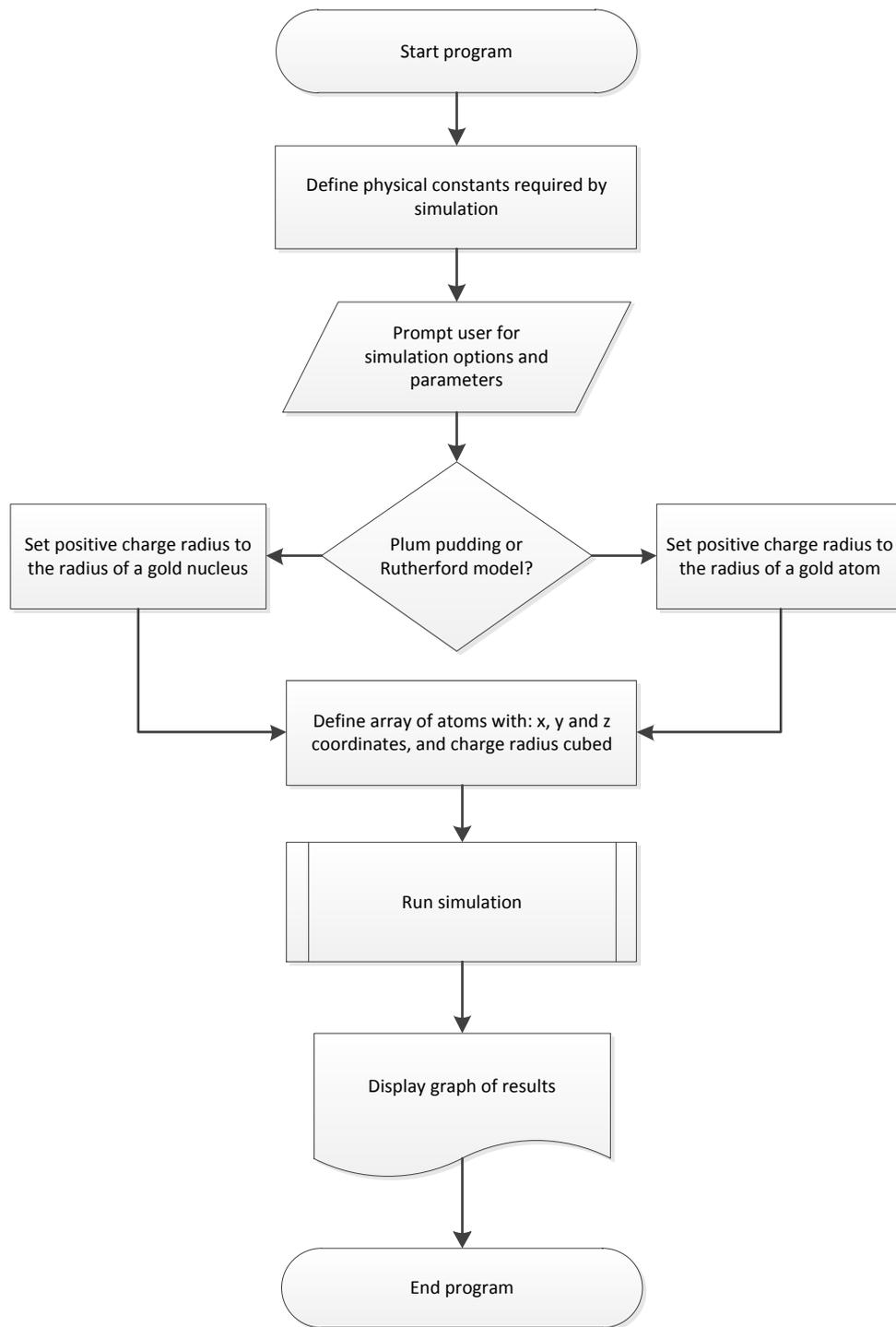


Figure 10:

Flowchart showing the main program flow of the alpha scattering simulation. The similarities with Figure 1 are clear. The “Run simulation” sub process also contains the core simulation logic and once again calls the ODEint function to perform the actual numerical integration required. Two similar sets of differential equations are used – one set for when an alpha particle is outside the charge radius of an atom and one when it is within. The result for the force inside a hollow shell is used, meaning that inside an atom there is less total force, since only the charge further exerts a net force, whereas the field due to the outer region disappears. Whilst outside of an atom, the effect of the electric field due to that atom is simply the same as for a point charge.

Scattering angles

The simulation was first set up to calculate the relationship between the angle of scattering by a single gold atom and the impact parameter. These results are shown below in figures 11 and 12. From this it is absolutely clear that a “plum pudding” atom as modelled cannot alone be responsible for any large angle scatterings. Although the simulation was later rewritten to model probabilities based on alpha particles being fired at random, these graphs provide the most visual evidence of the nature of the atom.

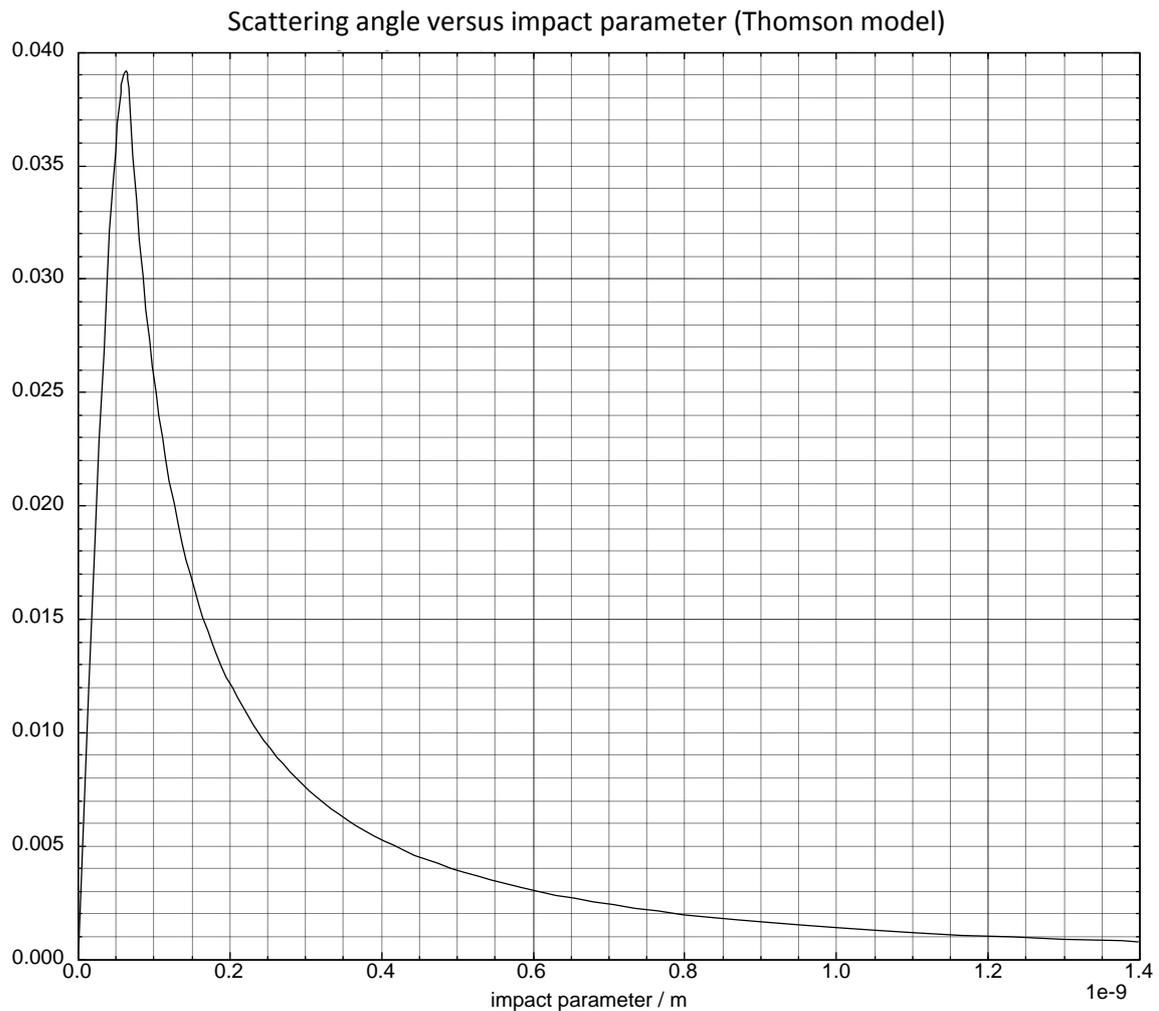


Figure 11:

The scattering due to a Thomson “Plum Pudding” atom (excluding the effect of any electrons) expressed as a relationship between scattering angle and the impact parameter of the collision. The largest possible scattering angle is less than 0.04 degrees, after which the angle of deviation drops off towards zero as the approaching alpha particles start further and further away from the atom.

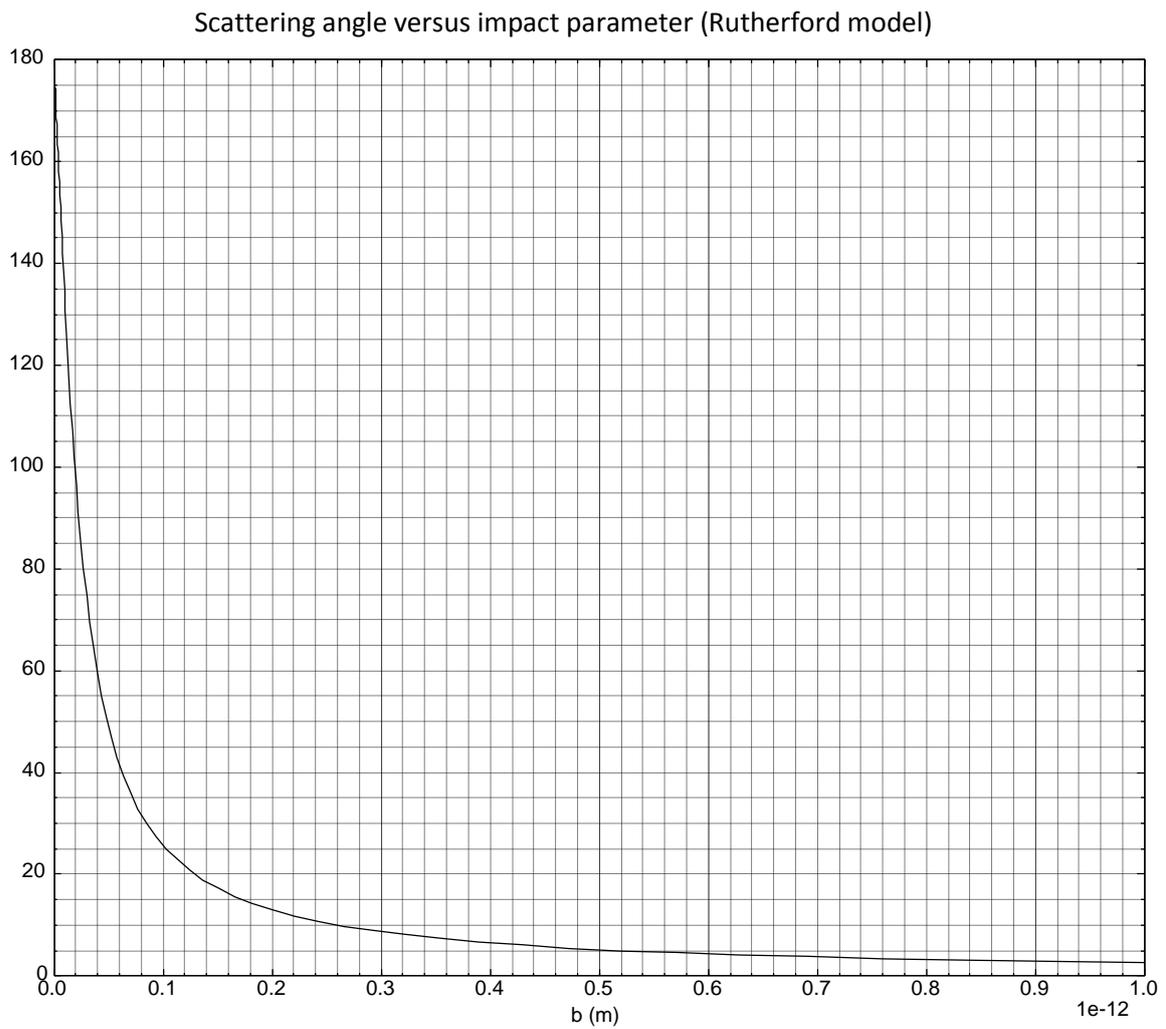


Figure 12:

Scattering angle versus impact parameter, b , for collisions between an alpha particle and a Rutherford “nuclear” atom (excluding the effect of any electrons). Huge scattering angles are possible up to 180 degrees, but only when the alpha particle approaches close to the tiny nucleus. After this, the angular deviation drops off quickly towards zero as the alpha particles start further and further away from the centre of the atom. In fact a long run of the simulation showed that only approximately 24 out of one million alpha particles were scattered by an angle of 5 degrees or higher by a single gold atom. To run the simulation with a lattice of atoms would take unfeasibly long, but is unlikely to provide very different results, since it is clear that the probability of multiple collisions is very small due to the size of the nucleus. This is shown analytically using statistical techniques in [3].

Conclusion

It has been shown that for a numerical model of a 2-d, two-body system, that the use of different coordinates has the effect of conserving the energy of the system to varying degrees. The conservation of energy has also been found to depend on the particular trajectories of the bodies, and thus on the system's initial conditions.

It is noted that gravitational effects are important for large masses over large distances, whereas atomic scales are very small. To further improve the numerical accuracy of the simulations, the units of each of the two systems could therefore be chosen such that the values of all coordinates are close to unity.

The reduced 2-body problem of the force on a single object due to another, larger, stationary object, was extended to a reduced 3-d, many-body system, using a simple algorithm consisting of nothing more than a summation. This is only possible because of the principle of linear superposition. However, the memory and computation time required to execute such a simulation, even for small numbers of particles, has been found to exceed the capacity of the average home PC. To run the simulation code as it stands would require a far more powerful computer and would take a considerable amount of time to run. It may be that an alternative algorithm could be used to reduce the computational resource required. Alternatively, it may be necessary to simplify the system by making further approximations, such as introducing a cut-off for the $1/r^2$ force at distances where it drops to a small enough value to be considered negligible.

References

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Appendix A – Satellite’s equation of motion in polar coordinates

To express the problem in plane polar coordinates, we use base unit vectors \hat{r} and $\hat{\theta}$, where:

$$\hat{r} = \cos\theta \mathbf{i} + \sin\theta \mathbf{j}$$

$$\hat{\theta} = -\sin\theta \mathbf{i} + \cos\theta \mathbf{j}$$

Choosing a frame of reference such that Mars is stationary and located at the origin, the satellite’s position is then given by:

$$\mathbf{r} = r \hat{r}$$

where r is the distance of the satellite from the centre of Mars.

Differentiating this expression gives the satellite’s velocity as:

$$\dot{\mathbf{r}} = \dot{r} \hat{r} + r\dot{\theta} \hat{\theta}$$

Finally, differentiating again gives the acceleration as:

$$\ddot{\mathbf{r}} = (\ddot{r} - r\dot{\theta}^2) \hat{r} + (2\dot{r}\dot{\theta} + r\ddot{\theta}) \hat{\theta} \quad [6]$$

Newton’s Law of Gravitation combined with his Second Law, gives the satellite’s equation of motion as:

$$\ddot{\mathbf{r}} + \left(\frac{GM}{r^2}\right) \hat{r} = \mathbf{0}$$

Combining this with the previous result gives the equation of motion in polar form:

$$\left(\ddot{r} - r\dot{\theta}^2 + \frac{GM}{r^2}\right) \hat{r} + (2\dot{r}\dot{\theta} + r\ddot{\theta}) \hat{\theta} = \mathbf{0}$$

where M is the mass of Mars.

This can also be written as a set of 1st order coupled ordinary differential equations by defining new variables such that:

$$v_{\theta} = r\dot{\theta}$$

$$v_r = \dot{r}$$

$$\dot{v}_r = \frac{v_{\theta}^2}{r} - \frac{GM}{r^2}$$

$$\dot{v}_{\theta} = -\frac{v_{\theta}v_r}{r}$$

Appendix B – Satellite's equation of motion in Cartesian coordinates

At any time, t , the satellite is at position \mathbf{r} and the force acting on it is:

$$\mathbf{F} = \frac{-GMm}{r'^3} \mathbf{r}'$$

where m is the mass of the satellite, M the mass of Mars and \mathbf{r}' is the displacement vector of the satellite relative to Mars, i.e.:

$$\mathbf{r}' = \mathbf{r} - \mathbf{R}$$

Therefore:

$$\ddot{\mathbf{r}} = \frac{-GM}{|\mathbf{r} - \mathbf{R}|^3} (\mathbf{r} - \mathbf{R})$$

Taking the y -axis such that Mars is moving with velocity:

$$\mathbf{V} = V\mathbf{j}$$

gives the position of Mars at t as:

$$\mathbf{R} = Vt\mathbf{j}$$

So, in Cartesian coordinates we can write:

$$\ddot{x}\mathbf{i} + \ddot{y}\mathbf{j} = \frac{-GM}{\left(\sqrt{x^2 + (Vt - y)^2}\right)^3} (x\mathbf{i} - (Vt - y)\mathbf{j})$$

Rewriting this as a set of coupled first order differential equations gives:

$$\begin{aligned}v_x &= \dot{x} \\v_y &= \dot{y} \\ \dot{v}_x &= \frac{-GMx}{\left(\sqrt{x^2 + (Vt - y)^2}\right)^3} \\ \dot{v}_y &= \frac{GM(Vt - y)}{\left(\sqrt{x^2 + (Vt - y)^2}\right)^3}\end{aligned}$$

Appendix C – Satellite’s equation of motion in Jacobi coordinates

In Newtonian mechanics, Jacobi coordinates are ideally suited for modelling two moving objects subject to no external forces. Physically, these coordinates represent the position of the centre of mass of the combined system and the separation between the individual centres of masses of the two objects. To model the motion of Mars and the satellite, we can define Jacobi variables as:

$$\mathbf{r} = \mathbf{r}_{Mars} - \mathbf{r}_{satellite}$$
$$\mathbf{R} = \frac{M\mathbf{r}_{Mars} + m\mathbf{r}_{satellite}}{M + m}$$

where M is the mass of Mars, m is the mass of the satellite, \mathbf{r}_{Mars} is the position vector of Mars and $\mathbf{r}_{satellite}$ is the position vector of the satellite.

It can then be shown that the equations of motion take on the simple form:

$$\ddot{\mathbf{r}} = -\frac{(M + m)G}{r^3}\mathbf{r}$$
$$\ddot{\mathbf{R}} = \mathbf{0}$$

These equations can also be split into Cartesian or polar components and expressed as a set of first order differential equations following a similar approach to those outlined in Appendices A and B.