PRACTICAL SESSION 1

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1 Fortran code to add an integer to a real number

In this first section we present a Fortran code that adds an integer to a real number and outputs the result to an external file. The code is the following:

2 Computation of Leibniz's formula

In this section we are going to use Leibniz's formula to compute the number π. The formula is the following:

$$\frac{\pi}{4} = \sum_{k=0}^{\infty} \frac{(-1)^k}{2k+1} \tag{1}$$

And the code used is the following:
As it can be seen, we set a maximum tolerance for the result, so that the loop keeps going until the error with respect to the exact value of π is smaller than such tolerance. In our case, this means () iterations.

3 Computation of the frequency spectrum S(ω)

In this section we are interested in computing the Fourier integral of a time-dependent correlation function $C(t) =< A(0)A(t) >$. Ignoring the normalization of the result, the expression is the following:

$$S(\omega) = \int_0^{\infty} C(t)cos(\omega t)\, dt \tag{2}$$

In order to make this calculation, we extract the $C(t)$ data, with time steps of $0.005ps$, from an external file named "corr.dat", and integrate the expression via Simpson's rule:

$$\int_a^b f(x)\, dx \approx \frac{\Delta x}{3} \left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{n-1}) + f(x_n)\right] \tag{3}$$

Where $\{x_0, \ldots, x_{n-1}\}$ are the $n+1$ points used in the integration, and $\Delta x = \frac{b-a}{n}$ is the step distance between such equiespaced points.
Furthermore, in order to obtain the frequency spectrum $S(\omega)$ we perform this integration for $\omega \in [0, 100]\, ps^{-1}$, for () different frequencies.
The code used is the following: The result obtained is shown below: As can be seen from the figure, this spectrum tells us that the most important frequency components are those around the peak observed at approximately $()\, ps^{-1}$.

4 Monte Carlo integration

In this section we are first looking to evaluate the area between the curves $y = x^{-1}$ and $y = -x^{-1}$ within the range $x \in [-1, 1]$ snd $y \in [-11, 11]$. The area to compute is represented in the following figure:
Secondly, we are interested in doing this integration for different total number of points N to analyze the method's precision by making use of the known exact result: $A_{exact} = 13.5916$. The N's we are going to use are $(100, 10^3, , 10^4, 10^5, 10^6, 10^7)$.
Furthermore, in order to perform a statistical analysis of the results, for every N we will compute the area $M = 100$ times, allowing us to obtain the mean value of the area ($< A(N) >$), and the standard deviation ($< \sigma(N) >$):

$$< A(N) >= \frac{1}{M} \sum_{i=1}^{M} A_i(N) \quad \& \quad < \sigma(N) >= \sqrt{< (A(N) - A_{exact})^2 >} \tag{4}$$

The code used is the following:
And the results obtained for the mean value and standard deviation of the area as a function of N and for $M = 100$ are:

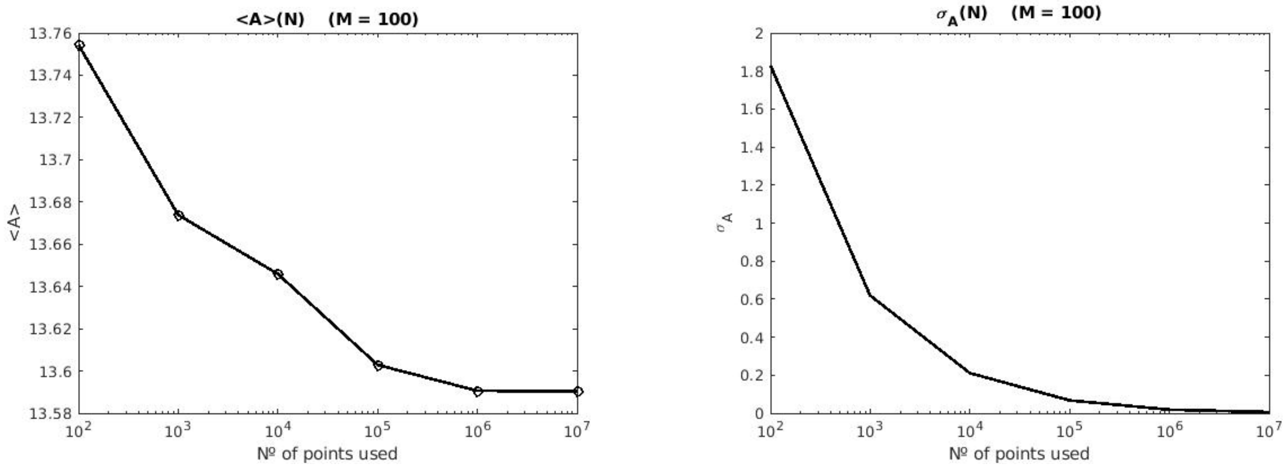

Figure 1: On the left, the mean value of A as a function of the number of points (N) used. And on the right, the standard deviation of such area.

5 Integration Algorithms

In this section we are going to analyze three different methods of integration for resolving equations of motion: Euler, Euler predictor-corrector and Verlet. In order to do this we are going to consider an harmonic oscillator of mass $m = 200\, g$ and force constant $k = 2\, N/m$, with initial position $x_0 = 5\, cm$ and $v_0 = 0\, m/s$.
To perform this analysis we will integrate the equations of motion via Euler's method using three different time steps:$\Delta t = 0.001\, s$, $\Delta t = 0.01\, s$ and $\Delta t = 0.02\, s$; via Euler's predictor-corrector method using $\Delta t = 0.02\, s$ and via Verlet's method using $\Delta t = 0.02\, s$.
This way we will compare the results of the three different time steps used in the computation via Euler's method, and compare the three different methods with $\Delta t = 0.02\, s$ with the exact analytical solution. This same analysis will be performed also for the comparison of the potential (U), kinetic (K) and total (E) energies. In this case we developed 4 different codes, one for each method and one for the exact analytical solution, each one yielding a file with the information needed to plot the results. The codes used are the following:
Having shown the code, the next step is to display the results. We start by showing in Figure 2 a comparison between the three different time steps used to solve the equation via Euler's method.

Next, in Figure 3 we show the trajectories obtained with the three different methods mentioned above when using a time step $\Delta t = 0.02\, s$ and compare them with the exact analytical solution. As it can be seen, Euler's method quickly diverges, and Euler's predictor-corrector and Verlet's method, are visually indistinguishable from the exact analytical solution. In order to show the difference more clearly, we plot, in Figure 4, each method's error with respect to the analytical solution.

We can then move on to the analysis of the energies obtained for each method with $\Delta t = 0.02\, s$. We start by displaying the kinetic energy (K) and the errors with respect to the exact solution in Figures 5 & 6. We follow by showing the same analysis for the potential energy (U) in Figures 7 & 8. And, finally, the results for the total energy (E) are shown in Figures 9 & 10.

From these results, we can conclude that Euler's method is by far the worst one, with Euler's predictor-corrector and Verlet's integration method yielding very similar results.

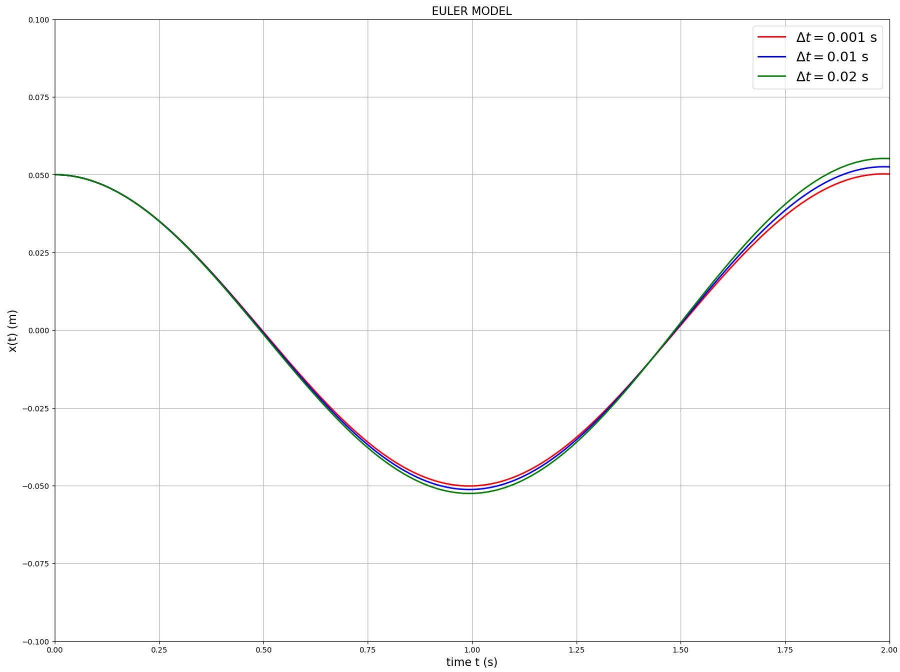

Figure 2: Trajectory obtained by solving the equation of motion via Euler's method with three different time steps: $0.001, s, 0.01s, and 0.02s$.

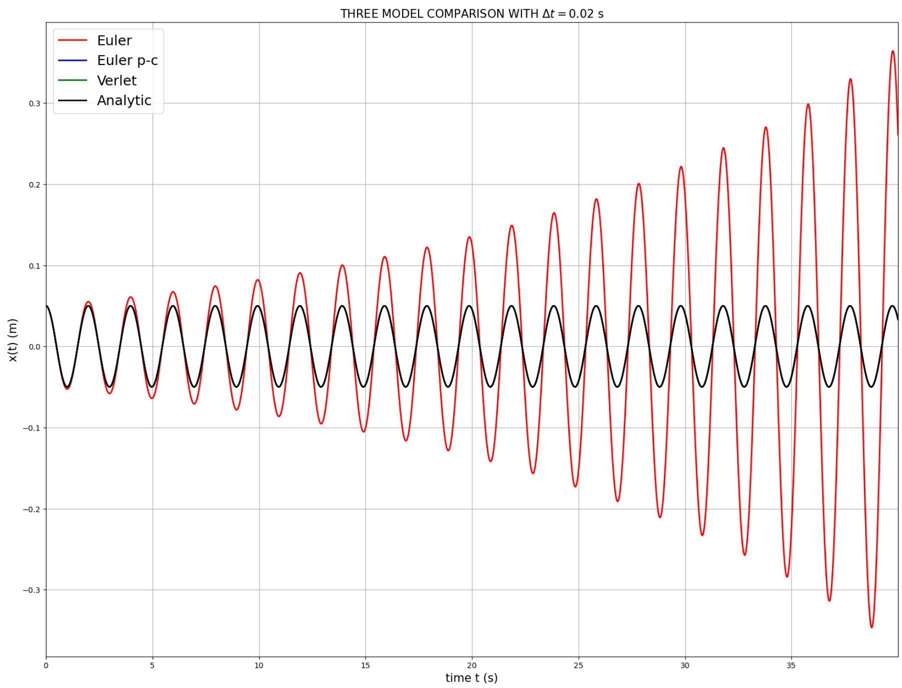

Figure 3: Trajectory obtained by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$, compared to the analytical solution.

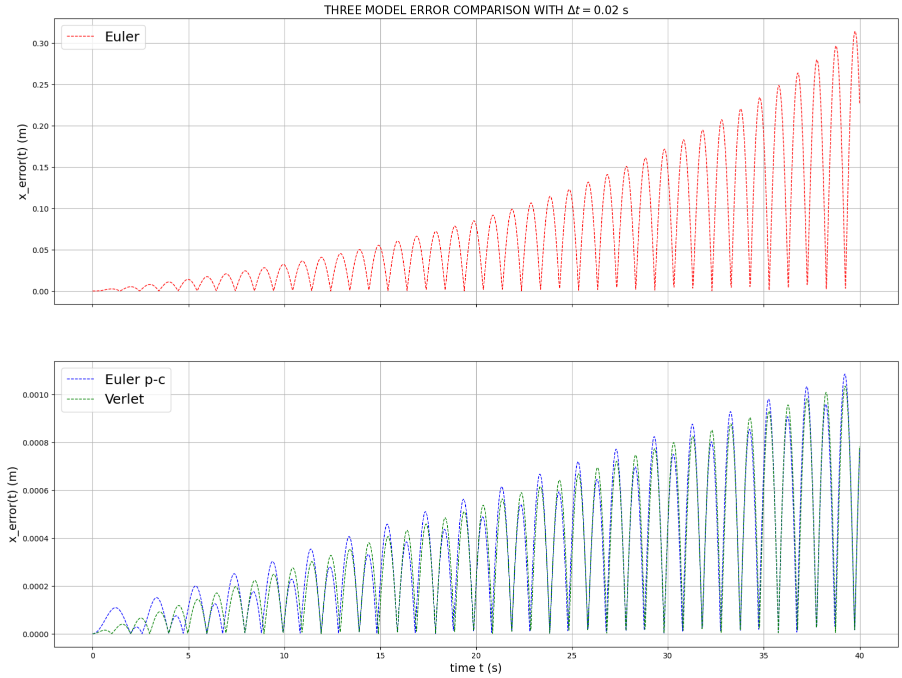

Figure 4: Errors obtained in the calculation of the trajectory by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

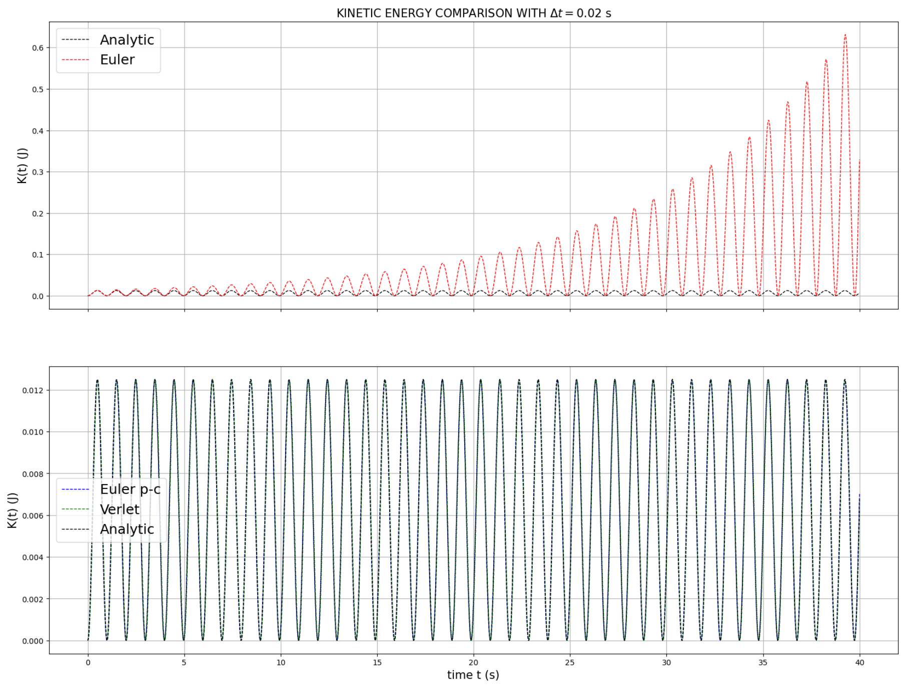

Figure 5: Kinetic energies obtained by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

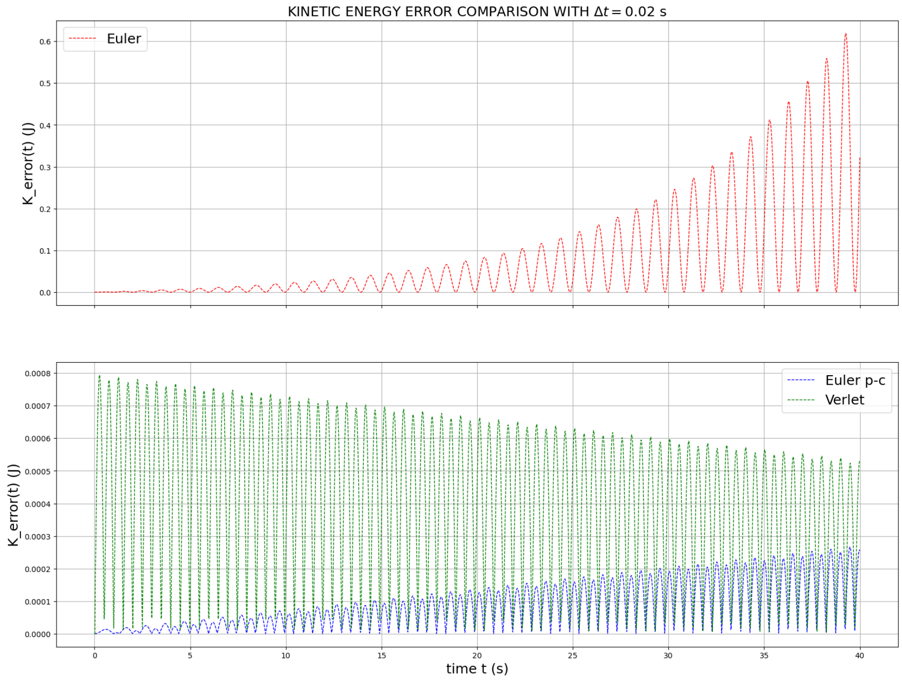

Figure 6: Errors obtained in the calculation of the kinetic energy by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

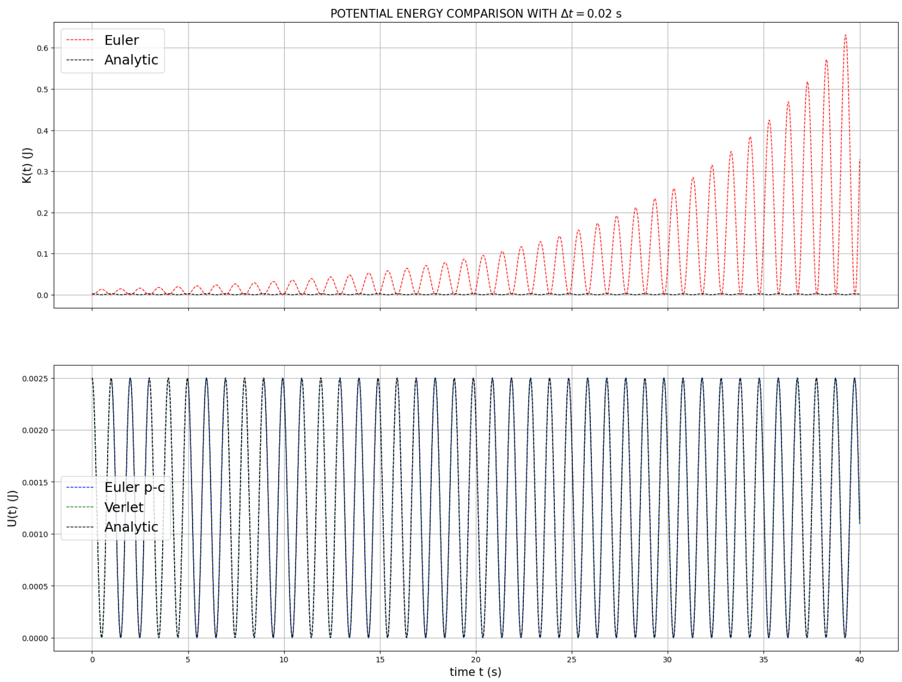

Figure 7: Potential energies obtained by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

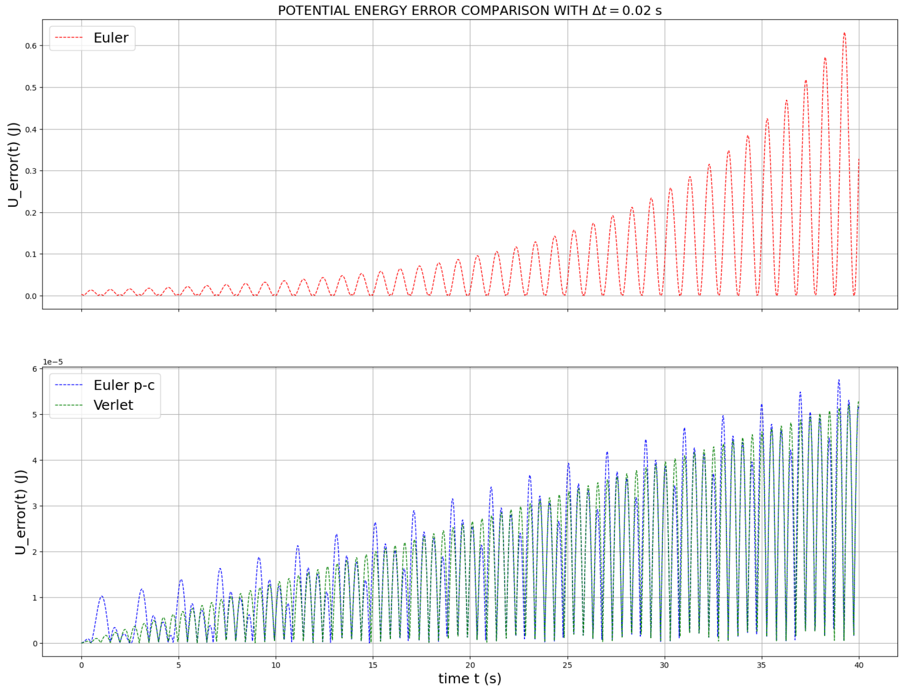

Figure 8: Errors obtained in the calculation of the potential energy by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

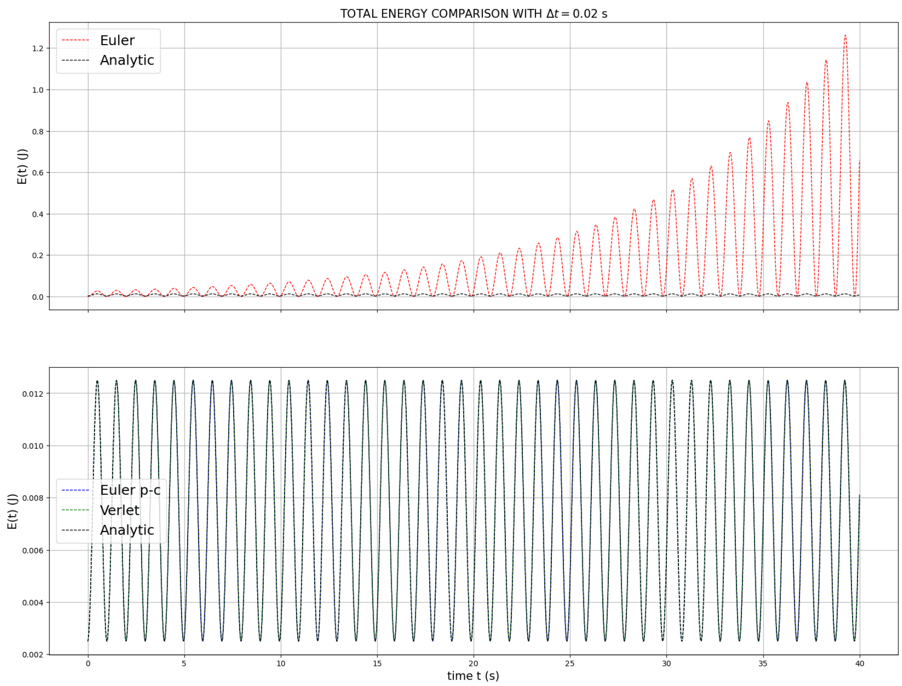

Figure 9: Total energies obtained by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.

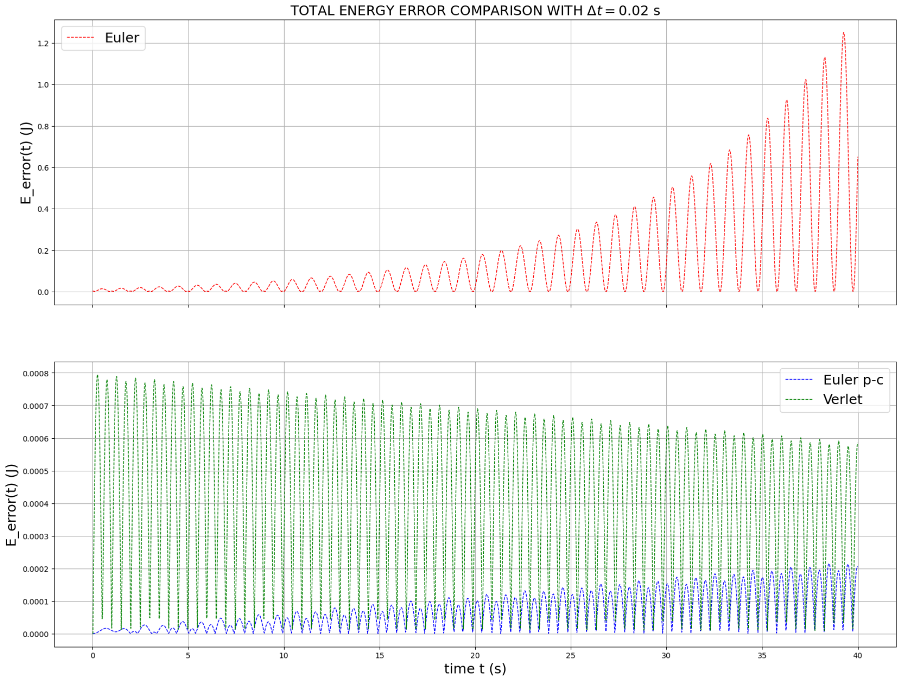

Figure 10: Errors obtained in the calculation of the total energy by solving the equation of motion via Euler's, Euler's predictor-corrector and Verlet's method with time step $\Delta t = 0.02s$ compared to the analytical solution.