Computer simulation in pysics

Harmonic oscillator analysis with different methods.

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Contents

List of Figures

1 Motivation

My motivation is to analyse the harmonic oscillator that tries to demonstrate a well-known problem in physics but now in English. We are in this University solved this problem in the first few weeks during the basic lecture and we used this example in the quantumechanics presentation in the last semester as well. So, this problem is following us to demonstrate all periodical motions. I show three different solutions of harmonic oscillation when i used Euler-Cromer , Euler and Runge-Kutta methods. I try to show the weakness of the methods and tried to find the borders of the modes and comparison with the well-known analytic solution.

2 Introduction and theoretical background

The three methods wherewith I worked used the basic oscillator equation, what we know from the Mechanics lecture:

$$\vec{F} = -D \cdot \vec{r}. \tag{2.1}$$

And after some transformation we can find the right solution for us to simulate the problem:

$$\frac{\partial^2 \vec{r}}{\partial t^2} = -\omega^2 \cdot \vec{r}, \tag{2.2}$$

Which can be traced back an attached system of differential equations

$$\frac{\partial \vec{r}}{\partial t} = \vec{v} \tag{2.3}$$

$$\frac{\partial \vec{v}}{\partial t} = -\omega^2 \cdot \vec{r} = \vec{a}. \tag{2.4}$$

And the analytic solution is:

$$r(t) = \vec{r_0} \cdot cos(\omega \cdot t) + \frac{\vec{v_0}}{\omega} \cdot sin(\omega \cdot t). \tag{2.5}$$

2.a Euler-Cromer and Euler methods

As we saw the attached system of differential equation (2.3, 2.4) we have to follow the same schema, but does not matter how.

At first look at the *Euler-Cromer* method.
If we have an initial *x(t=0)* diversion and a *t=0* starting velocity which we move with *dt* time steps, we get another attached system of equation for the time development:

$$v(t + dt) = v(t) + a(t)dt \tag{2.6}$$
$$x(t + dt) = x(t) + v(t + dt)dt \tag{2.7}$$

So with the *Euler-Cromer* method in the *2.7 equation* the velocity is evaluated at *t(t+dt)*. Advantage of this method that the energy of the motion is retained and take the below formula:

$$E = \frac{1}{2} \cdot m \cdot v^2 + \frac{1}{2} \cdot m \cdot \omega^2 \cdot x^2 \tag{2.8}$$

At the *Euler* method the velocity is evaluated at *t*. Which appear in the program code that we swap the two essential equations.
Because of this leap the energy in this method, it expands exponentially to infinity.

$$x(t + dt) = x(t) + v(t + dt)dt \tag{2.9}$$
$$v(t + dt) = v(t) + a(t)dt \tag{2.10}$$

Errors of the *Euler* method:

1. if the derivative changes too fast during the step, then step will have some error
2. over time, there will be a large deviation from the analytical solution
3. despite the error of the Euler method is $\mathcal{O}(h^2)$ however, the number of steps adds up to the error
4. if the step is halved, the error is reduced to a quarter, but twice as many steps are required.

2.b Runge-Kutta method

The *Runge-Kutta* method (RK45) is a method of the Runge-Kutta family. The essential technique is at each step, two different approximations for the solution are made and compared. If the two answers are in close agreement, the approximation is accepted. If the two answers do not agree to a specified accuracy, the step size is reduced. If the answers agree to more significant digits than required, the step size is increased. By performing one extra calculation, the error in the solution can be estimated and controlled by using the higher-order embedded method that allows for an adaptive step size to be determined automatically. The error of the Runge-Kutta method is $\mathcal{O}(h^5)$

Advantage of adaptive step size:

1. there is no need to estimate the step size, it is automatically guessed by the method
2. it moves very fast on the flat sections of the solution

Disadvantage of adaptive stepsize:

1. runtime cannot be estimated in advance
2. if the solution changes rapidly throughout, it slows down very much

The determination of coefficients is very hard. During the calculation of the coefficients is given by Butcher tables. Every method has an own Bucher table.

I used the Explicit Runge-Kutta method of order 5(4), what given by:

$$y_{n+1} = y_n + h \sum_{i=1}^{steps} b_i k_i \tag{2.11}$$

where k is:

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f(t_n + c_2 h, y_n + a_{21} h k_1), \\
k_3 &= f(t_n + c_3 h, y_n + a_{31} h k_1 + a_{32} h k_2), \\
&\;\;. \\
&\;\;. \\
&\;\;. \\
k_s &= f(t_n + c_s h, y_n + a_{s1} h k_1 + a_{s2} h k_2 + \cdots a_{s,s-1} h k_{s-1}).
\end{aligned}$$

3 Emphasize my contribution

3.a Euler method

I ran the program with seven different ω and the same initial conditions $x_0 = 0$ and $v_0 = 1$ as I mentioned in the theoretical background, we can see how the distance of the diversions is growing. We can see it with the green line the ratio of the difference to the analytic solution. As we expected the ratio and the analytic solution is in a linear relationship. The ratio is increasing exponentially. We can discover deviation in the ratio consistent grow on small scales, if we run the program with big ω, as we can see for example at 3.a.7.figure. That is also an observed phenomenon that we have already difference in the first period, and the maximum difference of distance is changes (3.d.1). Another result that we can see some period sliding (3.a.13.figure) if we use bigger ω. The energies of the motion as expected increases exponentially to infinity (3.a.16.figure).

<u>Distance</u>

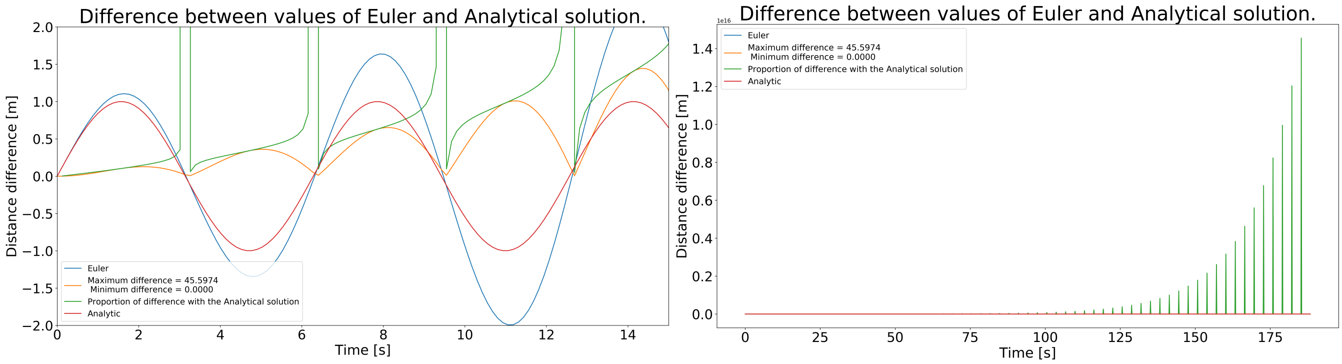

Figure 3.a.1:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 1$.

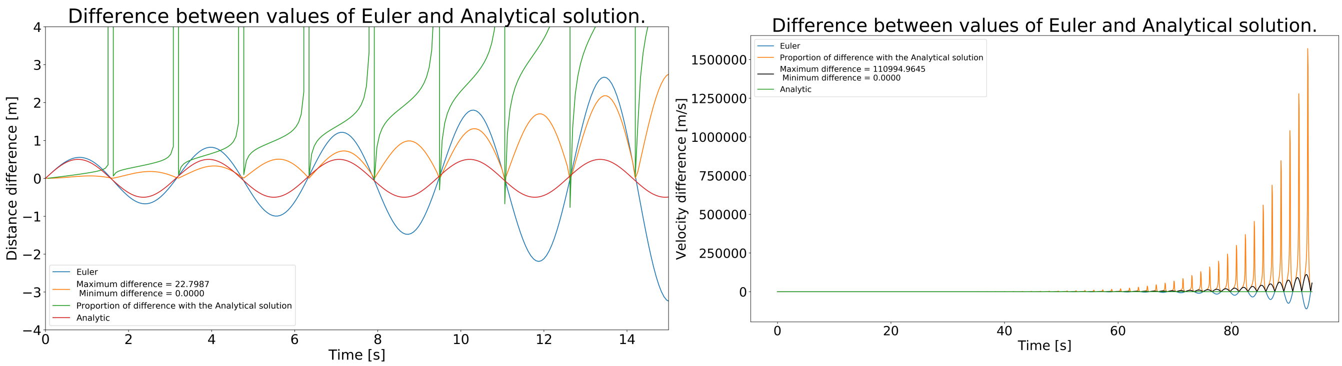

Figure 3.a.2:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 2$.

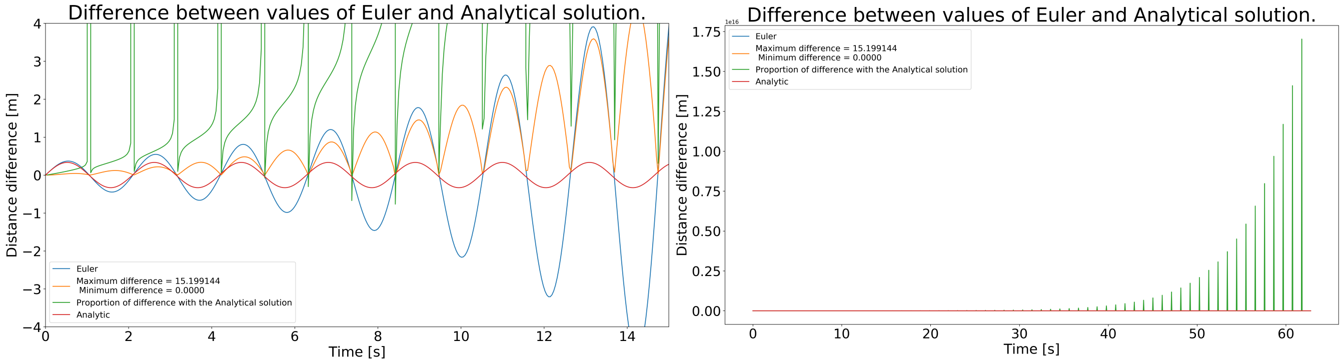

Figure 3.a.3:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 3$.

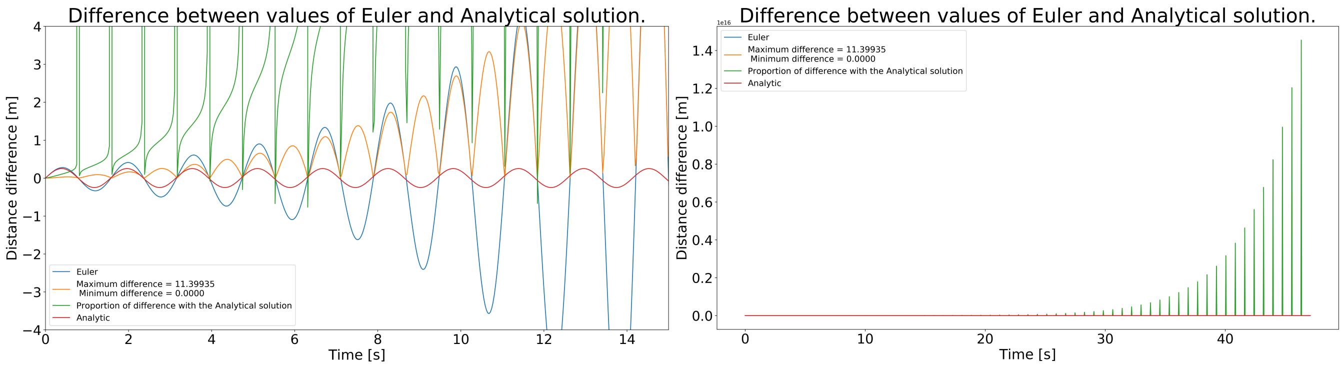

Figure 3.a.4:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 4$.

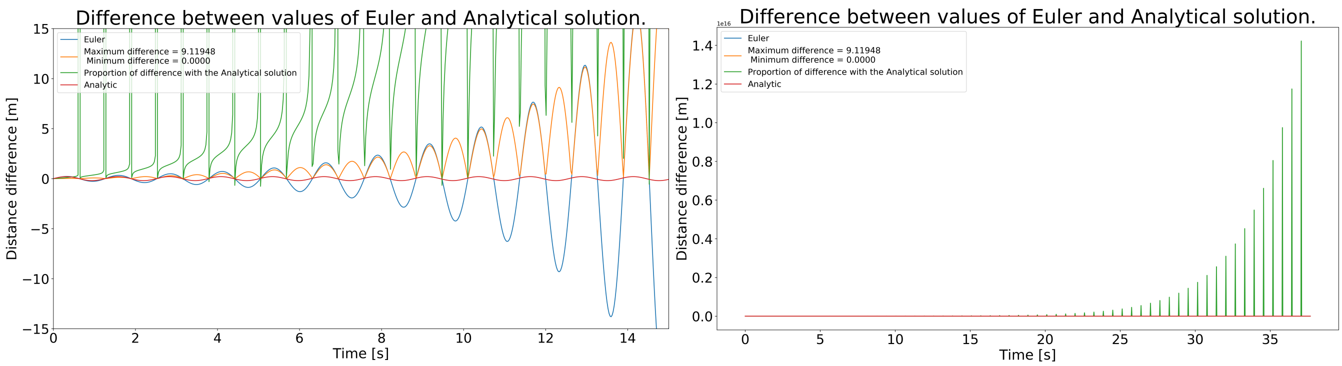

Figure 3.a.5:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 5$.

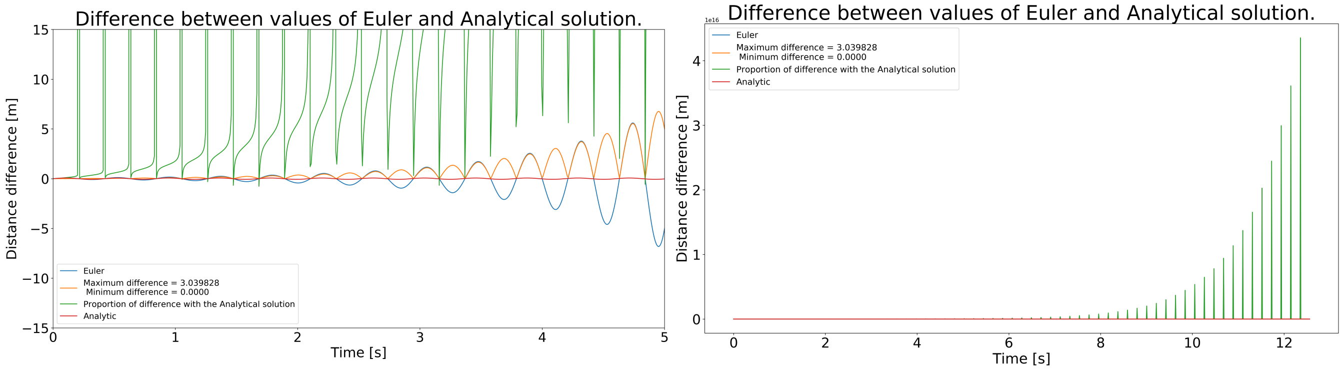

Figure 3.a.6:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 15$.

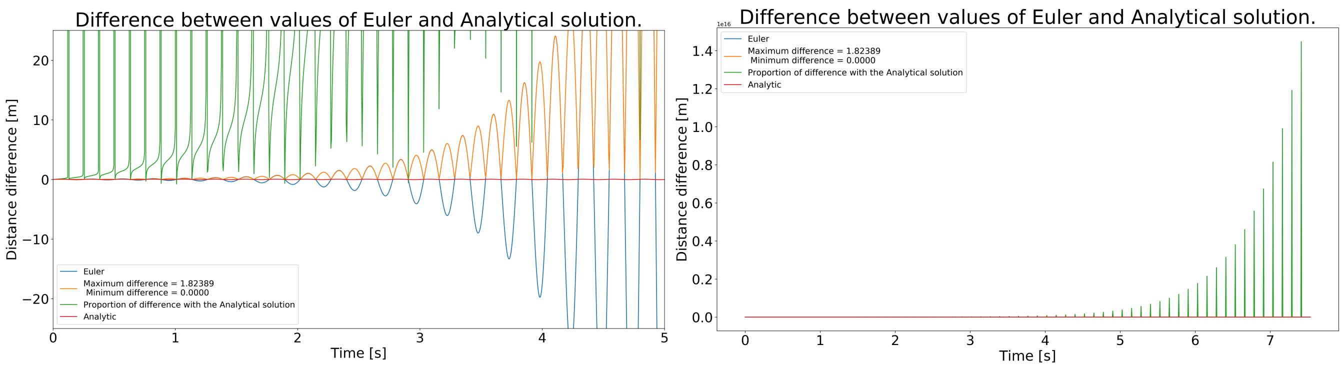

Figure 3.a.7:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 25$.

Velocity

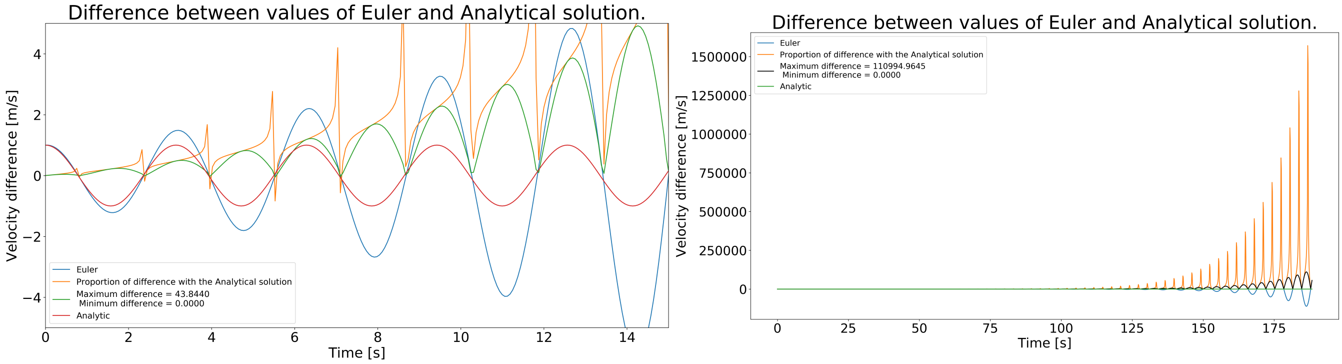

Figure 3.a.8:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 1$.

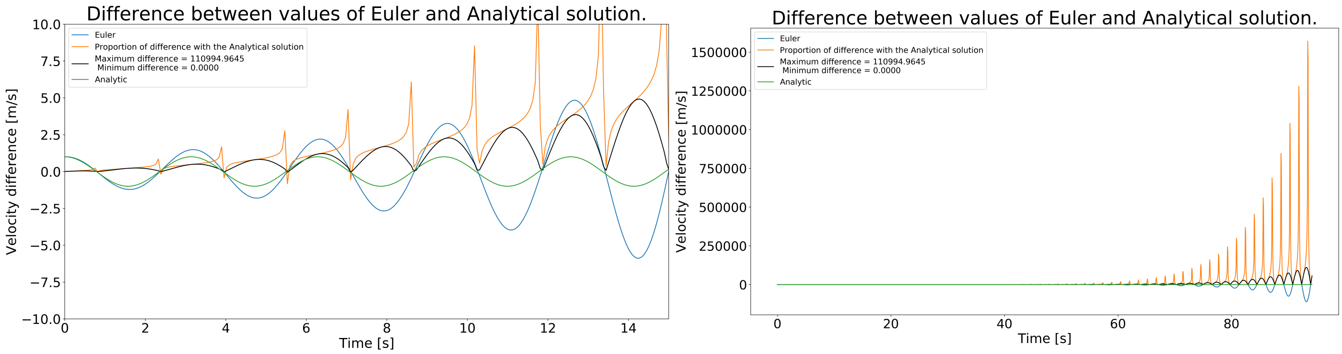

Figure 3.a.9:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 2$.

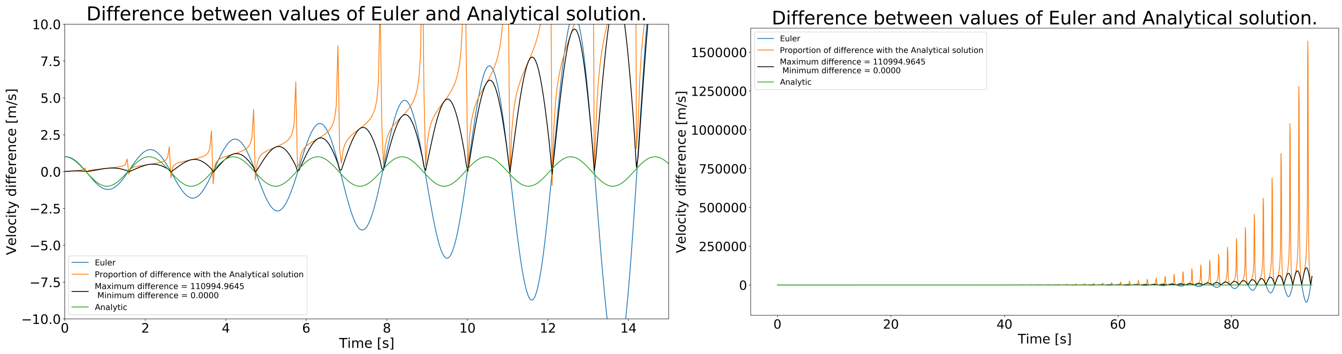

Figure 3.a.10:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 3$.

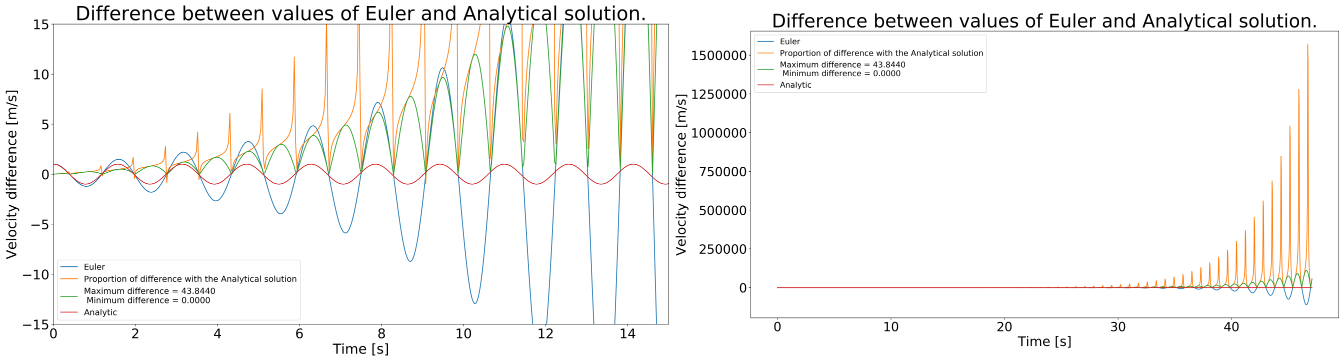

Figure 3.a.11:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 4$.

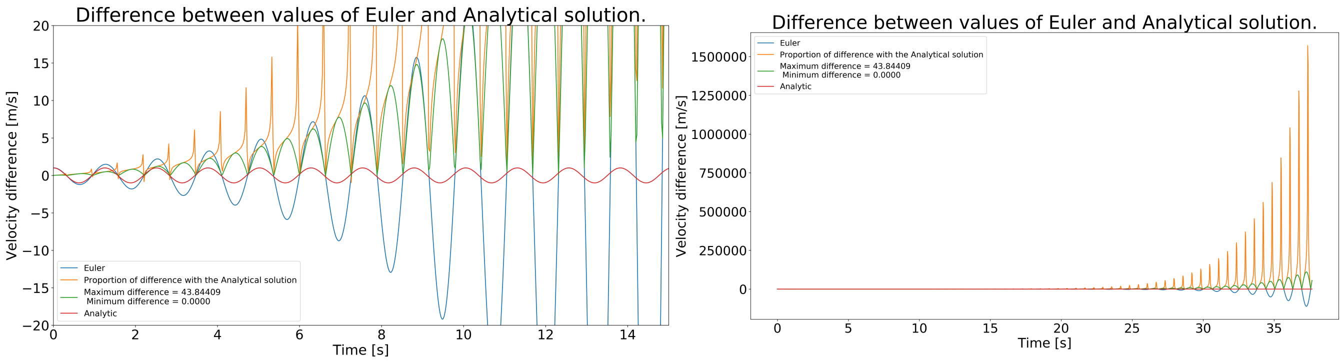

Figure 3.a.12:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 5$.

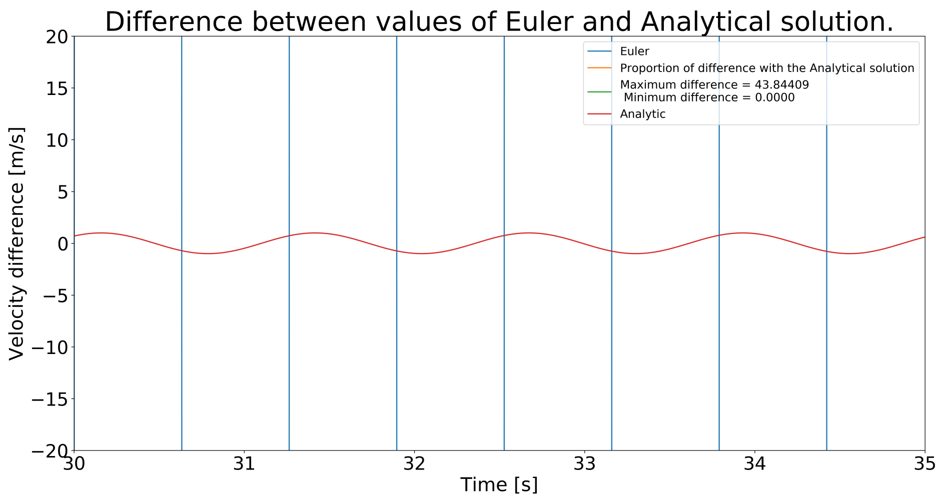

Figure 3.a.13:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 5$.

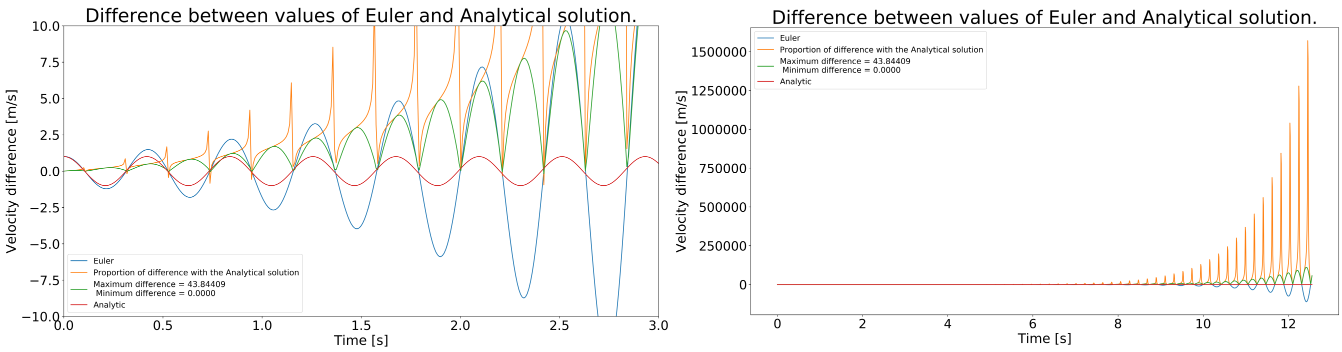

Figure 3.a.14:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 15$.

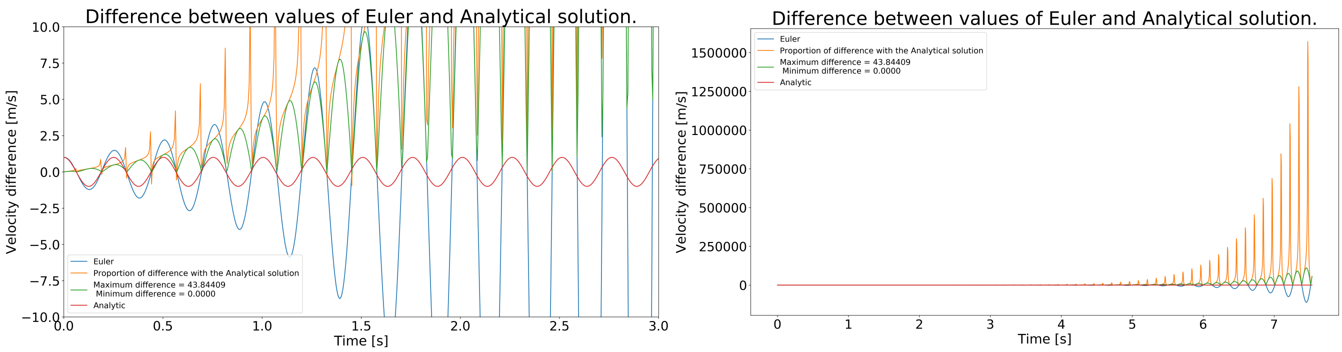

Figure 3.a.15:
Velocity and velocity difference between values of Euler and Analytical solution, $\omega = 25$.

Energy

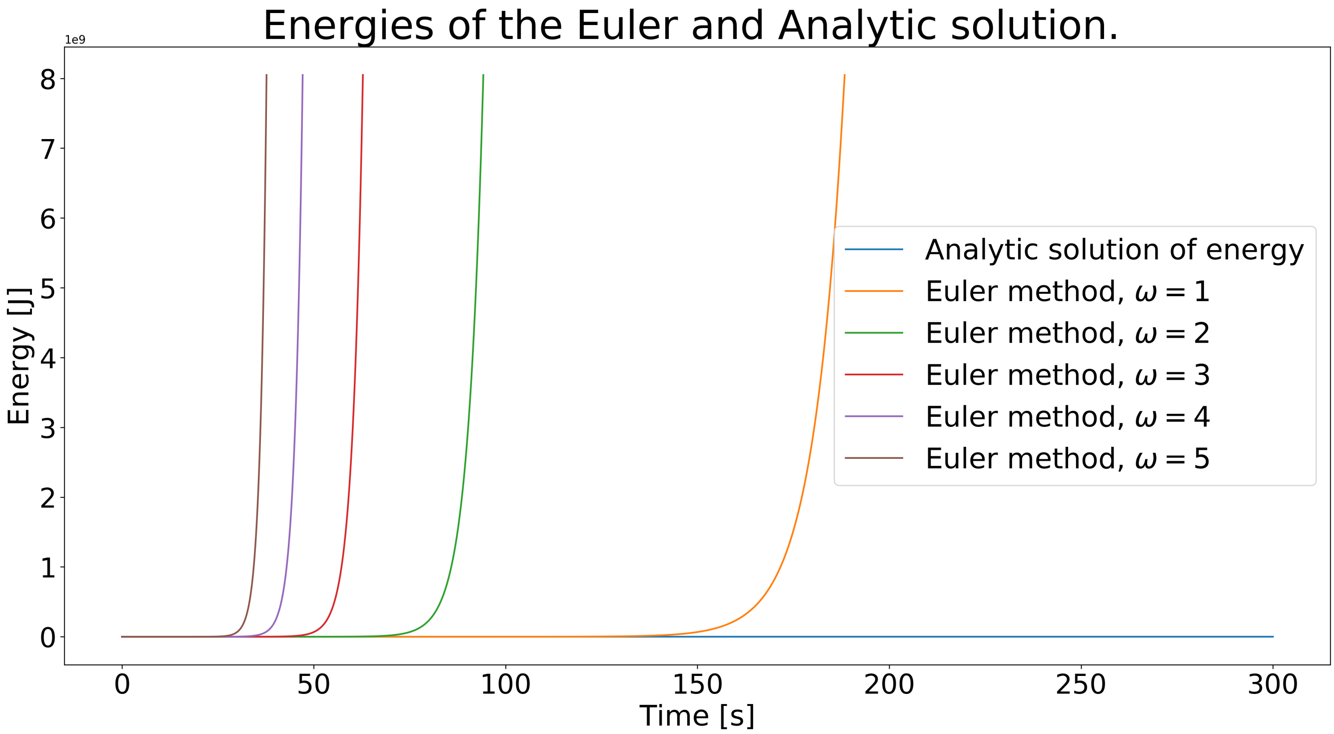

Figure 3.a.16:
Energies of Euler method solutions.

3.b Euler-Cromer method

In the figures we can see (from 3.b.1 to 3.b.6), if we compare between analytic and Euler-Cromer solutions of same ω-s that with constant step size and with growing ωs the two signs have a gap. We can decrease the gap of the signs if we decreased the step size. Of course, the main question here is which one method is cheaper, whichever is more cost effective. In the figures with yellow we can see the two sign's ratio of the difference to the analytic solution, we can see the lines are in a linear relationship. The ratio is increased linearly. The increases is faster for larger ωs but if we connect the maximum of periodic deviations, and see that as a line the slope is constant. The lines of velocities we can see a pattern. The two sign's ratio of the difference to the analytic solution is decrease, so somewhere in the middle of the period examined the two signs is the same. As we know from our studies that energy must remain at the harmonic oscillator. This is clear from the values calculated by the Euler-Cromer (3.b.14.figure). At this method also have changes in the maximum difference of distance (3.d.2.figure), but now smaller with two orders of magnitude.

<u>Distance</u>

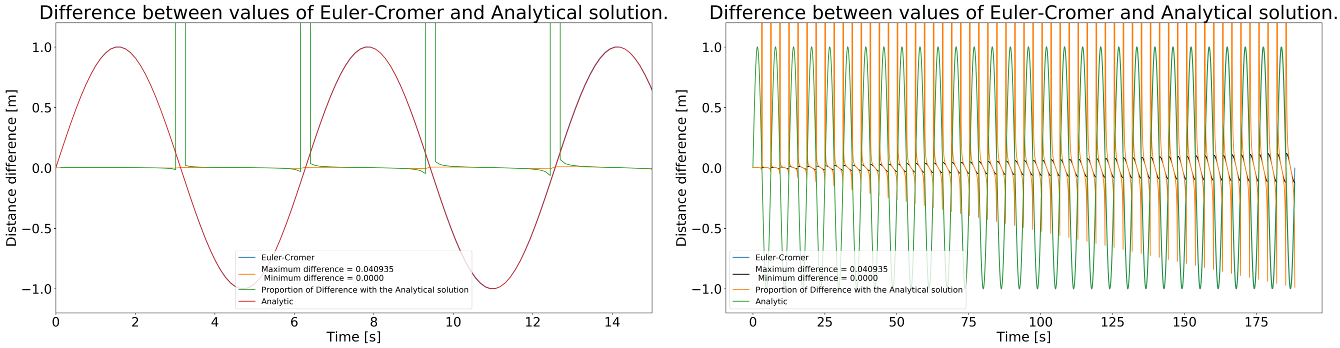

Figure 3.b.1:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 1$.

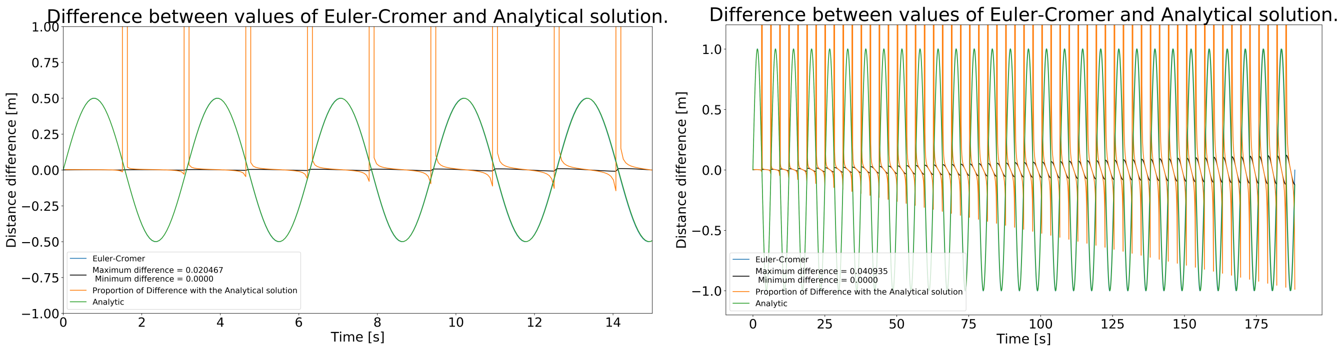

Figure 3.b.2:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 2$.

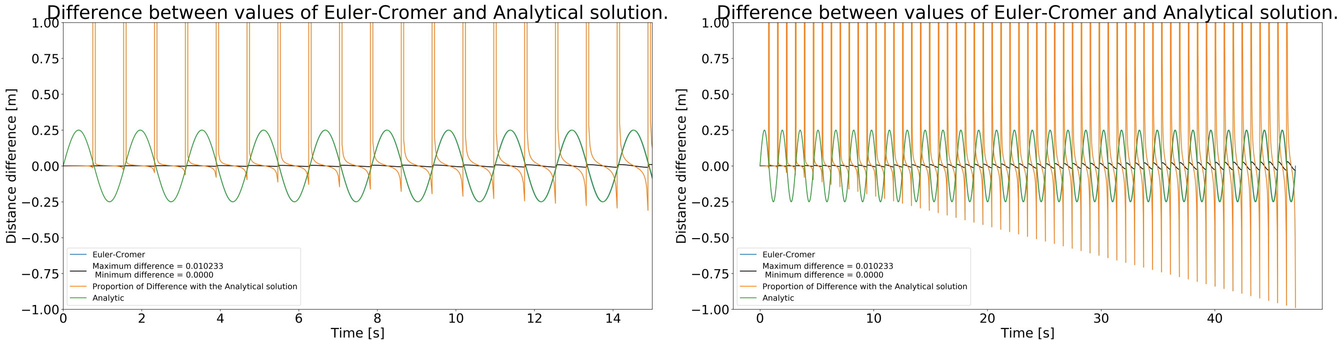

Figure 3.b.3:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 4$.

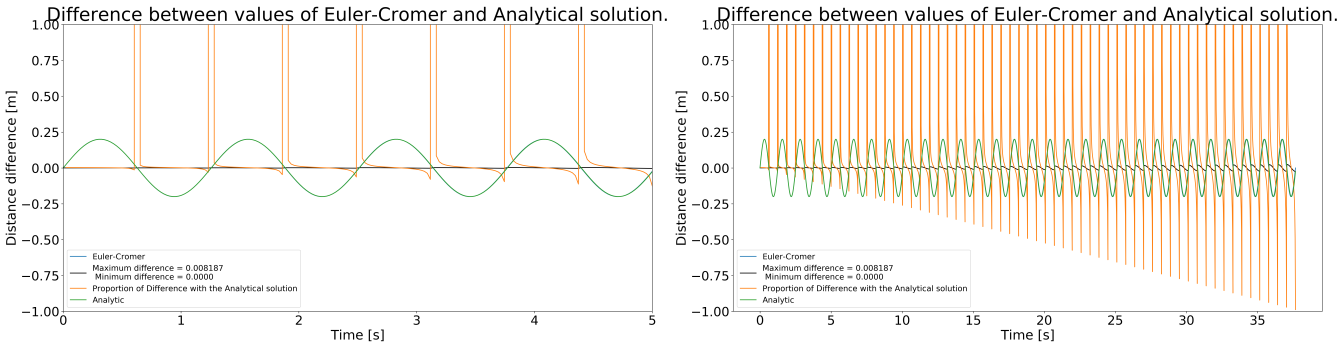

Figure 3.b.4:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 5$.

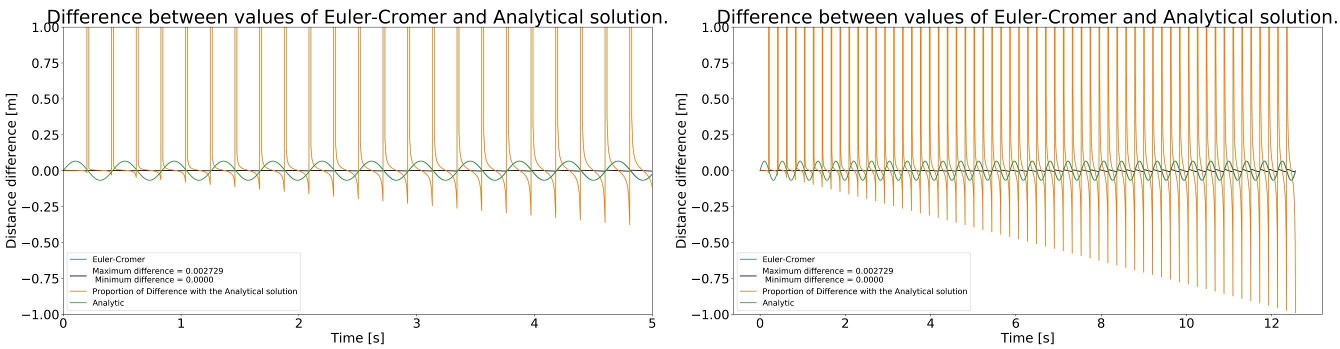

Figure 3.b.5:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 15$.

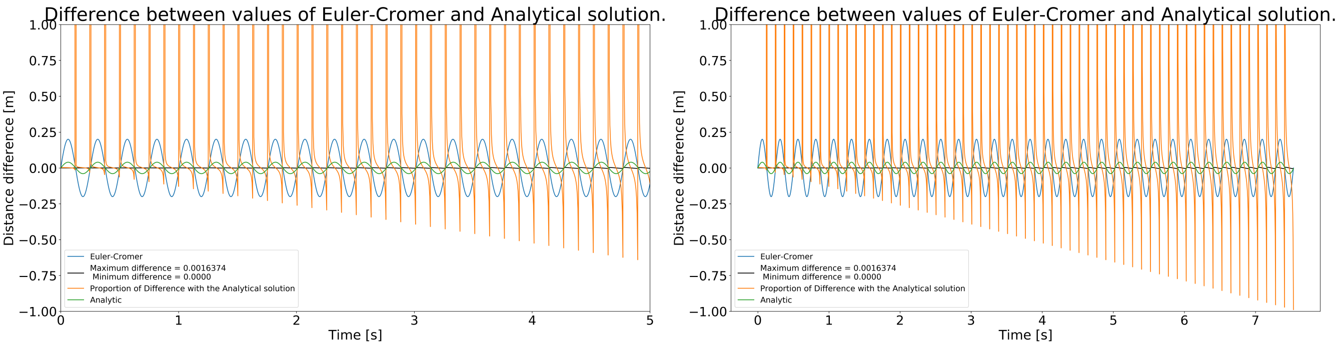

Figure 3.b.6:
Distance and difference of distance between values of Euler and Analytical solution, $\omega = 25$.

Velocity

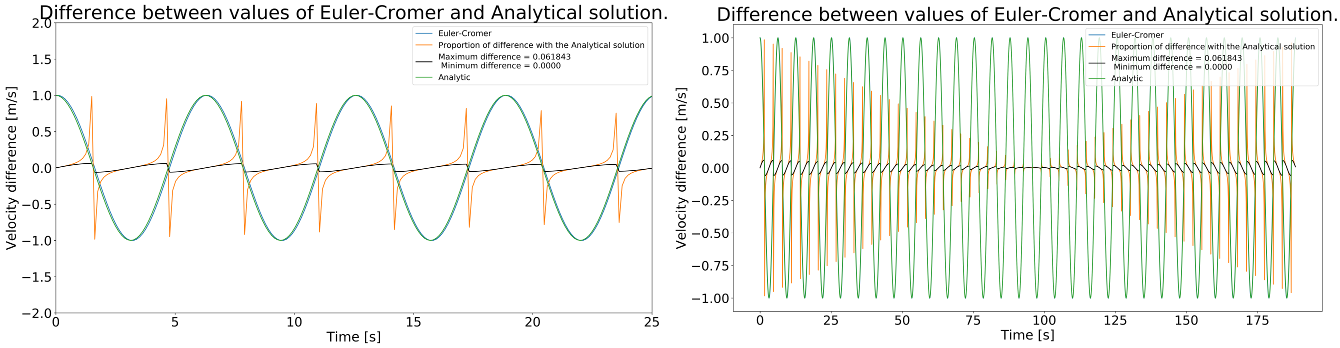

Figure 3.b.7:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 1$.

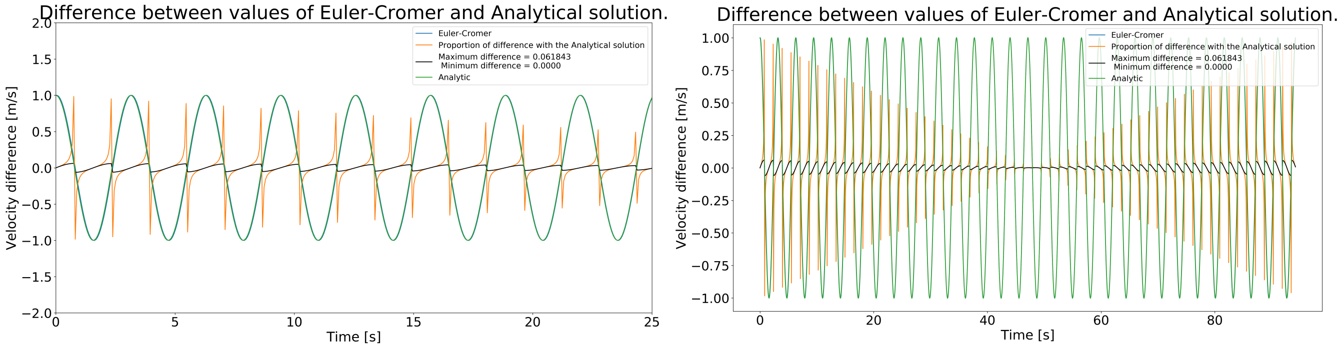

Figure 3.b.8:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 2$.

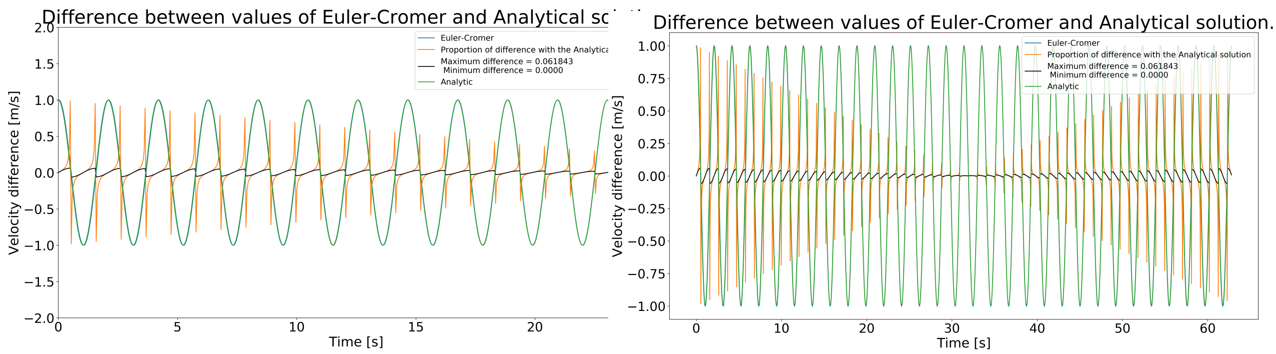

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Figure 3.b.9:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 3$.

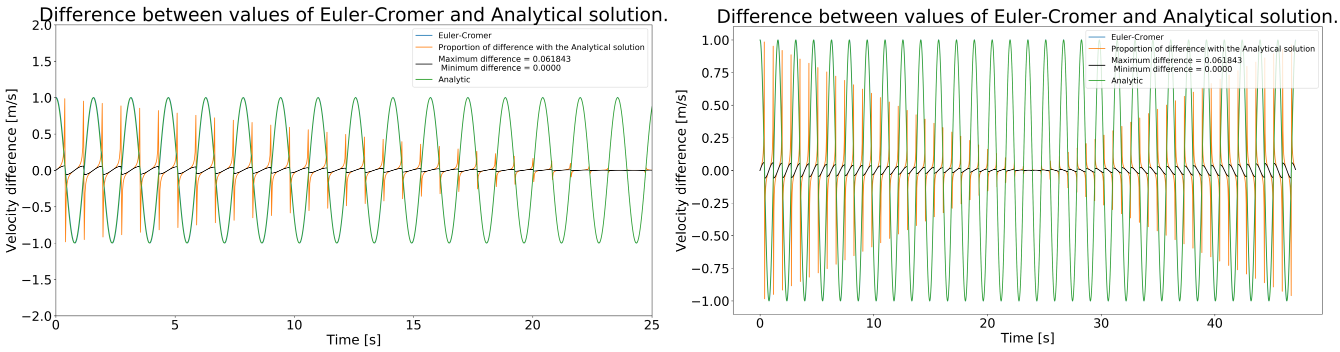

Figure 3.b.10:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 4$.

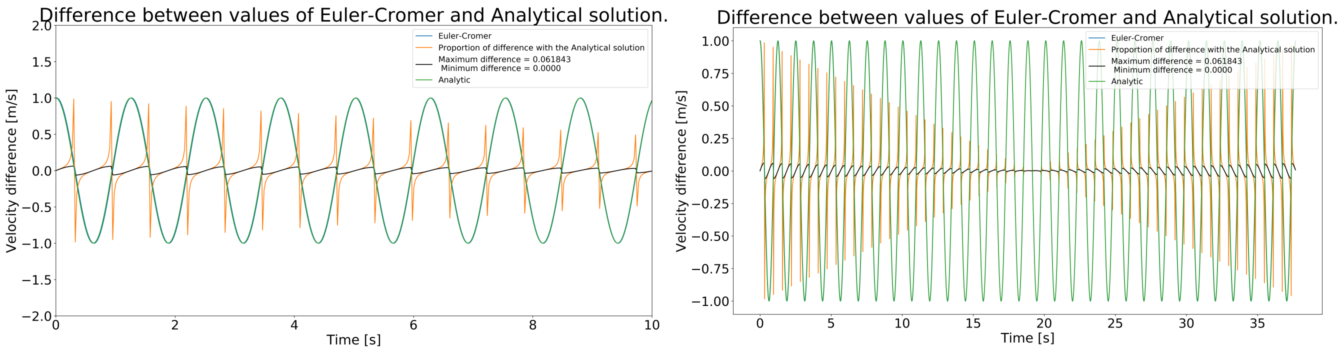

Figure 3.b.11:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 5$.

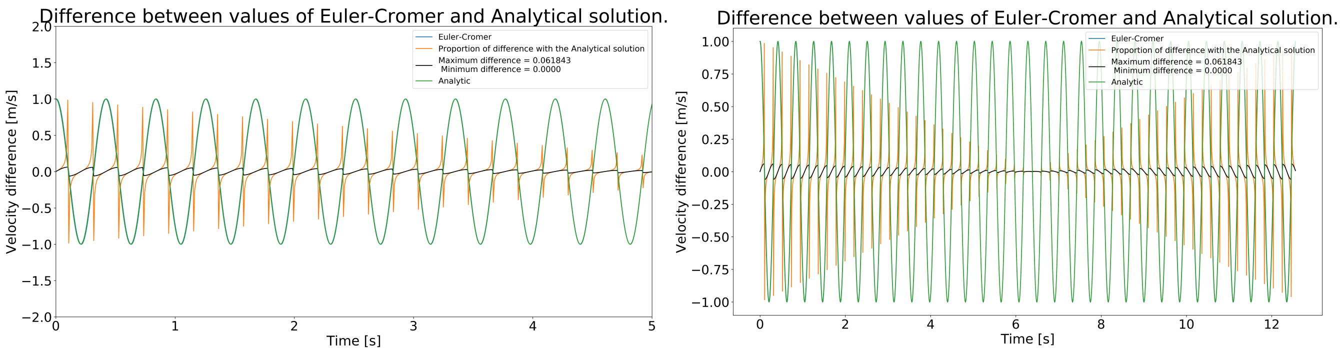

Figure 3.b.12:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 15$.

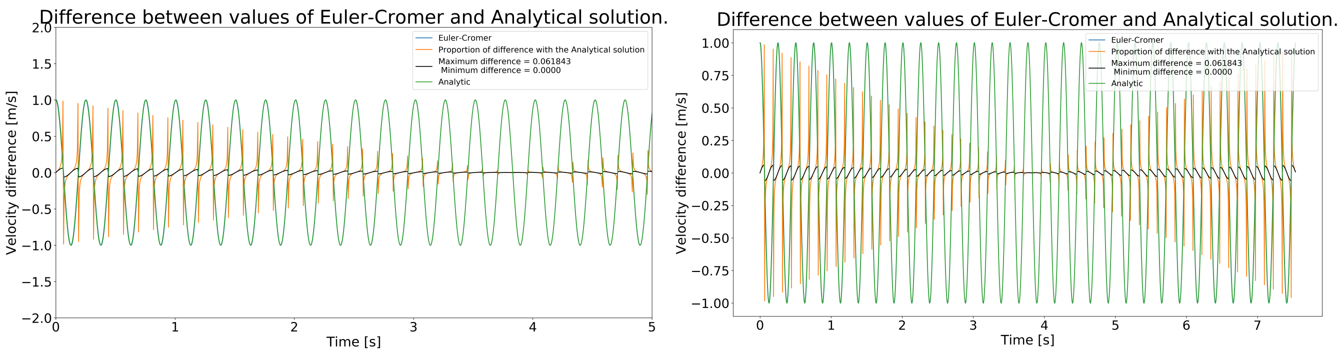

Figure 3.b.13:
Velociy and velocity difference between values of Euler-Cromer and Analytical solution, $\omega = 25$.

Energy

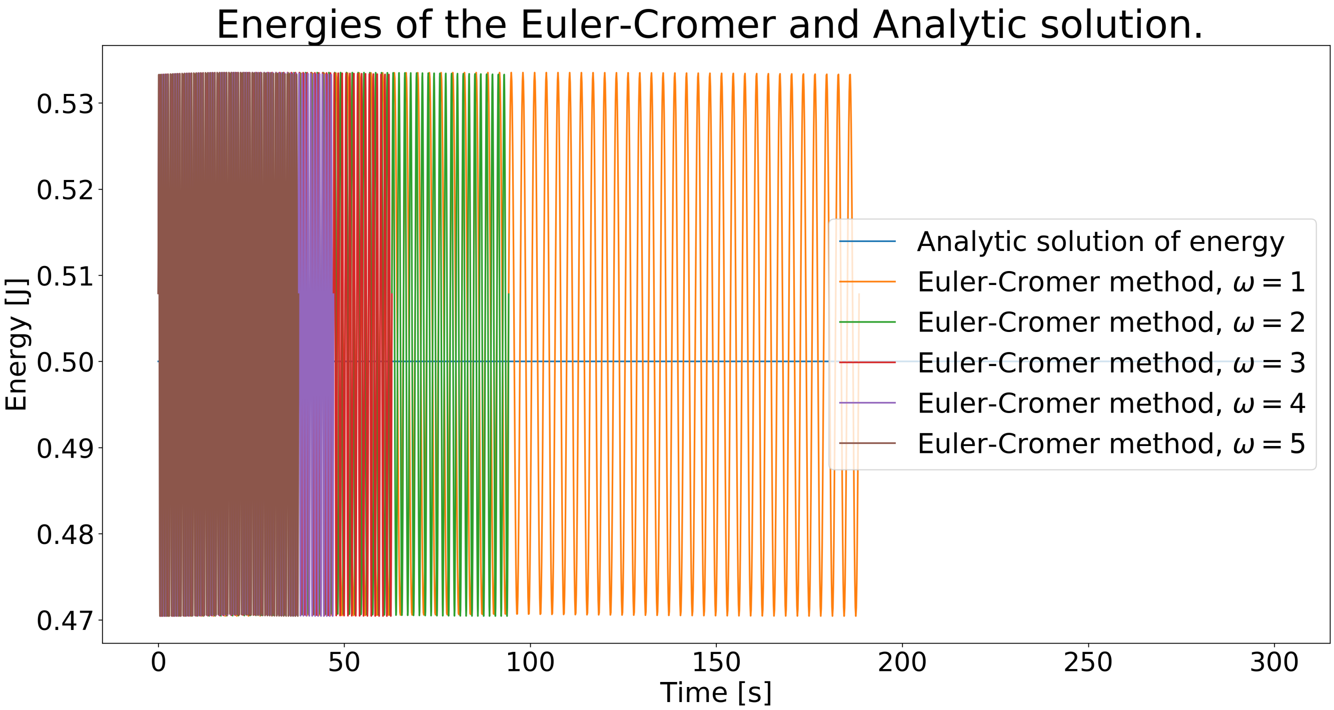

Figure 3.b.14:
Energies of Euler-Cr method solutions.

3.c Runge-Kutta method

We can do the most accurate simulations with this method if we have enough memory in the computer. But in the figures we see, we have always differences between the two signs.

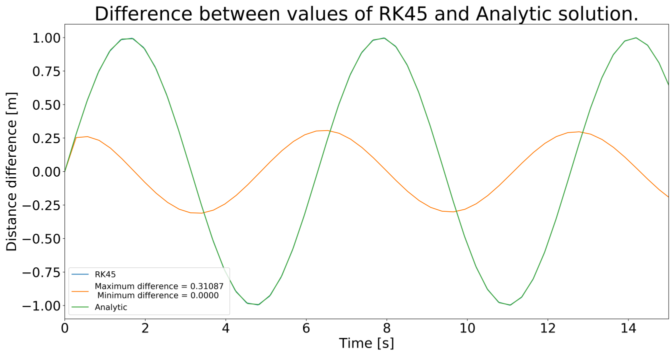

Figure 3.c.1:
Distance and distance difference between values of Runge-Kutta and Analytical solution.

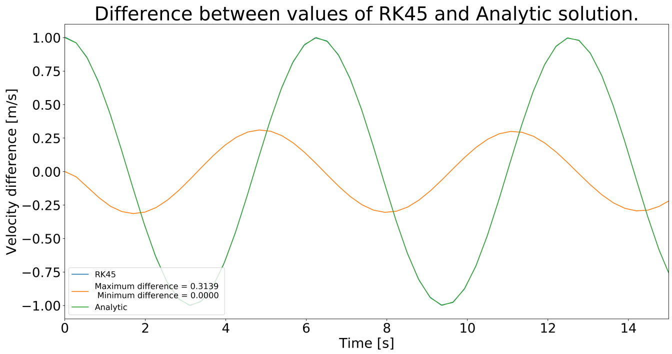

Figure 3.c.2:
Velocity and velocity difference between values of Runge-Kutta and Analytical solution.

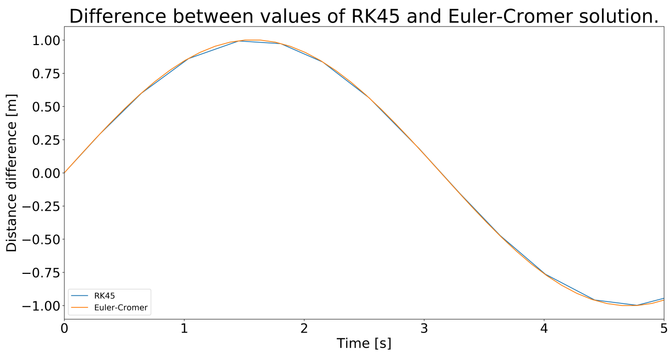

Figure 3.c.3:
Distance and distance difference between values of Runge-Kutta and Euler-Cromer solution.

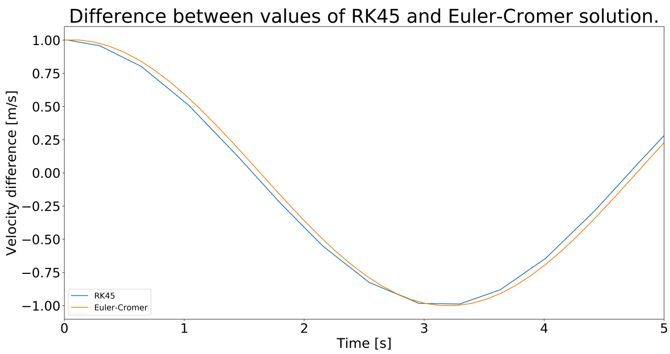

Figure 3.c.4:
Velocity and velocity difference between values of Runge-Kutta and Euler-Cromer solution.

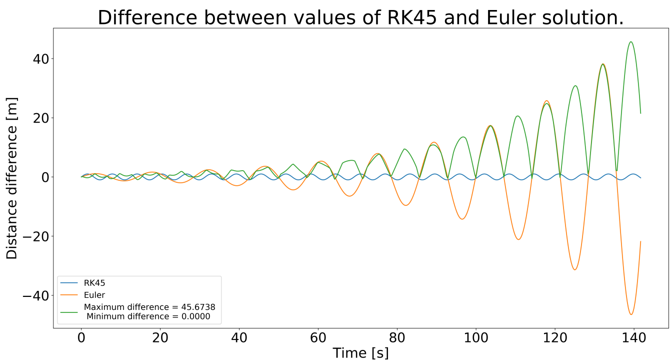

Figure 3.c.5:
Distance and distance difference between values of Runge-Kutta and Euler solution.

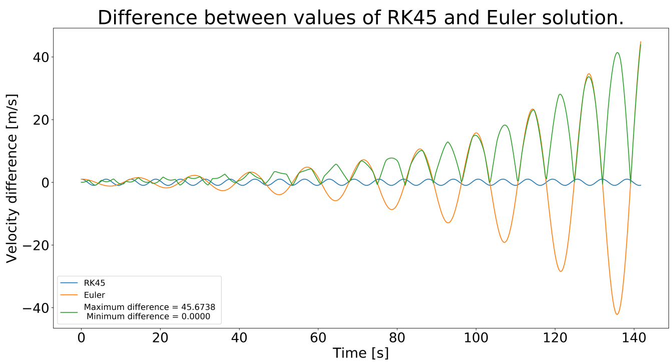

Figure 3.c.6:
Velocity and velocity difference between values of Runge-Kutta and Euler solution.

3.d Differences

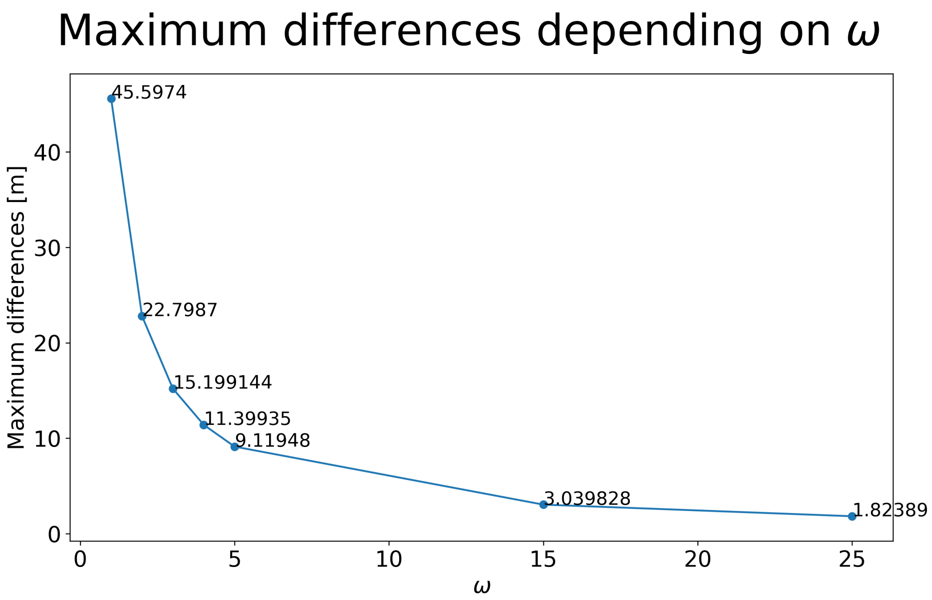

Figure 3.d.1:
Maximum different depending on ω used by Euler method

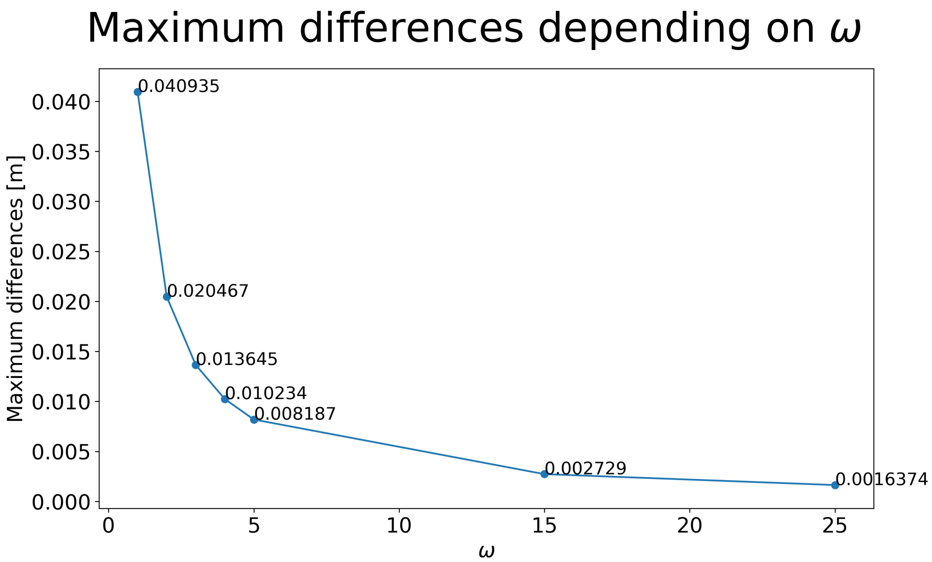

Figure 3.d.2:
Maximum different depending on ω used by Euler-Cromer method

3.e Phase space

With the Euler method we can see how could be more precise of the solution if we are increases the steps (3.e.2.figure), so we can approach the analytical solution on the phase diagram.
With Euler-Cromer method we can see with purple the same ω and step size line the analytic solution and we discovered a distortion on the circle, we can explain this with the little peak what appearing every half period (3.b.8.figure), what comes from the two sign's ratio of the difference to the analytic solution.
With RK45 we can see how insecure the solution. But if we have enough data to calculate the average of the values it can be a good solution as well.

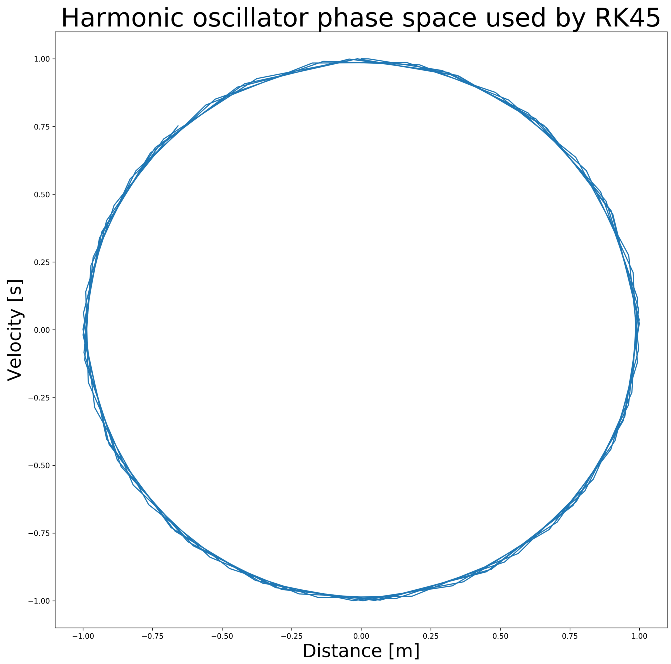

Figure 3.e.1:
Phase space used by RK45 method.

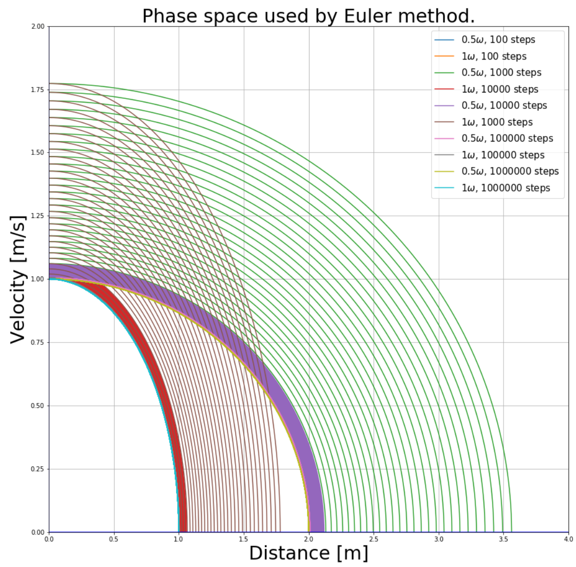

Figure 3.e.2:
Phase space used by Euler method.

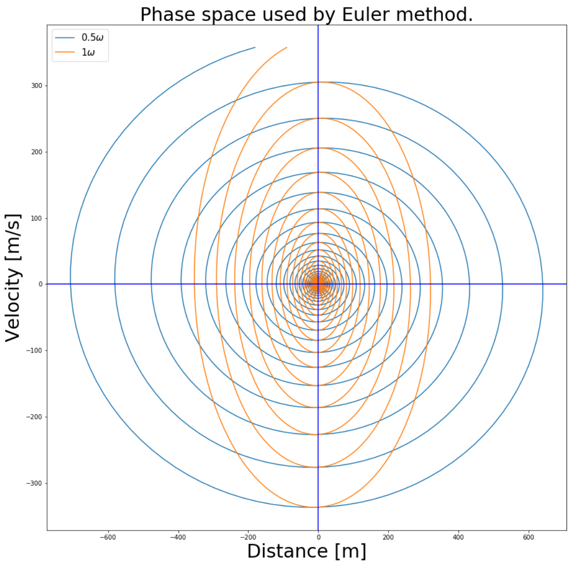

Figure 3.e.3:
Phase space used by Euler method.

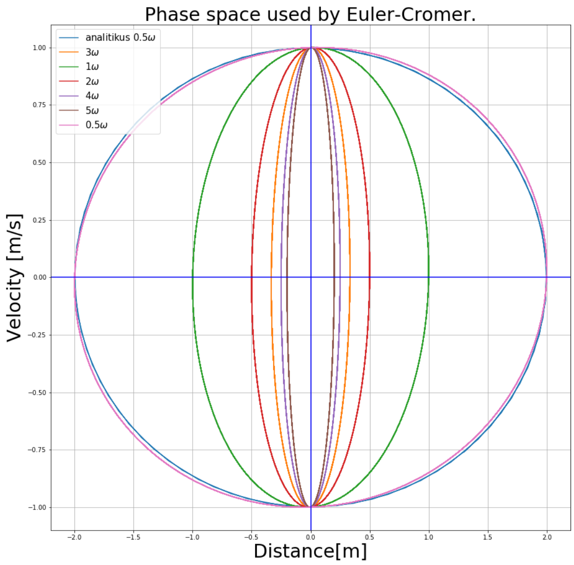

Figure 3.e.4:
Phase space used by Euler-Cromer method.

4 Discussion

Euler method:

- we can prove the theoretical background,
- the ratio and the analityc solution are in a linear relationship. The ratio is increasing exponentially,
- deviation in the ratio consistent grow on small scales,
- we have already difference in the first period,
- the maximum difference of distance is changing,
- slip period,
- if we increases the steps we can approach the analytit solution in phase space.

Euler-Cromer method:

- we can prove the theoretical background,
- the ratio and the analytic solution are in a linear relationship. The ratio is increasing linearly,
- the increases is faster for larger ω but if we connect the maximum of periodic deviations, and see that as a line the slope is constant.
- changes in the maximum difference of distance , but smaller with two orders of magnitude than Euler method,
- the distortion on the circle comes from the difference to the analytic solution.

Runge-Kutta:

- we can prove the theoretical background,
- The widest scalable simulation, but strong computer needed,
- insecure solution if no appropriate step is set.

5 Conclusion

Both simulation methods are good for work, but does not matter which is the goal. It was a mistake from me, that is not added timer for the codes to examine the runtime, because from the time we could calculate that which one is worth it better. But I think if we have data from Runge-Kutta method and we calculate the average of those, we could not make a big mistake and that one is the fastest.