Integration Project

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1 Introduction

The two physics problems studied in this project were a damped spring-mass system and the probability density of a particle in a box(PIAB).

1.1 Damped Spring-Mass System

The damped spring-mass system was represented as a second order ordinary differential equation (ODE) with no external force acting on the system. A particular spring-mass system with mass m, a damping constant of c, a spring force constant of k and an equilibrium length of x=0 can be modeled using Eq. 1 shown below:

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0 \tag{1}$$

Analytically solving this equation requires finding the roots of the characteristic equation using the quadratic equation as shown below:

$$mr^2 + cr + k = 0 \implies r = \frac{-c \pm \sqrt{c^2 - 4mk}}{2m} \tag{2}$$

The general solution for Eq. 1 is written in the form:

$$x(t) = e^{\alpha t}(c_1 cos(\beta t) + c_2 sin(\beta t)) \tag{3}$$

where rearranging Eq. 2 to the form $\alpha + i\beta$ provides their respective values for a specific solution as shown below in Eq. 4

$$r = \frac{-c \pm \sqrt{c^2 - 4mk}}{2m} = \frac{-c}{2m} \pm i\sqrt{\frac{k}{m} - \frac{c^2}{4m^2}} \tag{4}$$

Depending on the value of c the spring's motion can be described as falling into one of four categories: no damping, under damping, critically damped, and over damped. Graphs displaying each of these behaviors will displayed in the following sections.

1.1.1 No Damping

In the case where there is no damping, $c = 0$ and the roots of the characteristic equation are equal to $\pm$i $\sqrt{\frac{k}{m}}$ yielding the general solution:

$$x(t) = c_1 cos(\sqrt{\frac{k}{m}}t) + c_2 sin(\sqrt{\frac{k}{m}}t) \tag{5}$$

This describes a harmonic oscillator that will continue to oscillate indefinitely with a fixed amplitude since there is no term decreasing the displacement of the spring as time goes on

1.1.2 Under Damping

In the case where there is under damping, c is not 0 and so as time progresses the spring's motion is inhibited until eventually reaching the equilibrium position. This time the roots of the characteristic equation are $\alpha + i\beta$ yielding the general solution:

$$x(t) = e^{\frac{-c}{2m}t}(c_1 cos(\sqrt{\frac{k}{m} - \frac{c^2}{4m^2}}t) + c_2 sin(\sqrt{\frac{k}{m} - \frac{c^2}{4m^2}}t)) \tag{6}$$

Since α is non-zero, as time goes on the exponential term drives the displacement of the spring back to 0.

1.1.3 Critical Damping

In the case of critical damping, the spring is driven back to the equilibrium position as quickly as possible and does not undergo any oscillations. This situation occurs when $c^2 = 4mk$ causing the discriminant in the quadratic equation to equal 0, leaving us with one repeated root of $\frac{-c}{2m}$. This causes the general solution to take the form of

$$x(t) = c_1 e^{\frac{-c}{2m}} + c_2 t e^{\frac{-c}{2m}} \tag{7}$$

1.1.4 Over Damping

Lastly, in the case of over damping, the spring is driven back to the equilibrium position and does not undergo any oscillations. This behavior appears to behave similarly to critically damping except that it takes a longer time to reach the equilibrium position. This situation occurs when the discriminant is positive and causes the general solution to the take the form of

$$x(t) = c_1 e^{r_1} + c_2 e^{r_2} \tag{8}$$

1.2 Probability Density of 1D-PIAB

The normalized probability density function of particle confined to a one-dimensional box of length L and quantized energy level n can be described by the analytical function below

$$P(x) = \frac{2}{L} sin^2(\frac{n\pi x}{L}) \tag{9}$$

This function allows for determining the probability density of finding this quantum particle at position x within the box.

In this 1D-PIAB model the allowed energy levels are positive integers but the length of the box can be any positive value. In addition the probability of finding the particle within (0,L) is equal to 1 and so the integral across this region will always be equal to 1.

2 Integration Algorithms

Various integration algorithms were implemented on both damped spring-mass system and the probability density function and later compared against preexisting algorithms.

2.1 ODE Methods

2.1.1 Euler's Method/Explicit Method

The first integration method tested was Euler's method or the explicit method, which approximates the next value of a function by using the previous value and derivative with respect to time at the previous value as shown in the equation below:

$$x_{t+1} = x_t + \frac{dx}{dt}dt \tag{10}$$

where $\frac{dx}{dt}$ represents the spring-mass's velocity at time t.In addition, since this systems velocity changes with respect to time, the updated velocity can be expressed in a similar way to position as shown below:

$$v_{t+1} = v_t + \frac{vx}{dt}dt \tag{11}$$

This method's solution can be compared to the analytically determined solution as seen in Figure 1 with the specified parameters listed below. In this case the spring is in an under damped situation and oscillates back and forth until eventually landing back to the equilibrium position. However it is clear that the explicit solution's displacement graph oscillates from greater displacement's than the analytical solution's graph and takes longer to return to the equilibrium position.

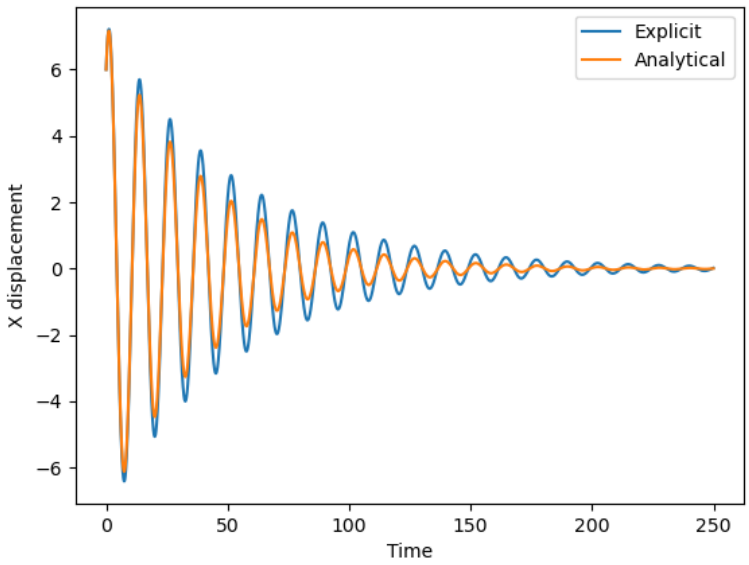

Figure 1: Plot comparing the analytical function and the explicit solution with a mass of 20kg, spring with force constant of 5N/m, damping constant of 1 Ns/m, initial displacement of 6m, initial velocity of 2m/s and time step of 0.05s

2.1.2 4th Order Runge-Kutta Method

The second integration method tested for the damped-spring problem was the fourth order Runge-Kutta method. This method determines the next value of the position function based on the previous position, the particular time step and a weighted average of 4 slopes across this time step. In the damped spring problem, the slope of the position graph is determined by the velocity and so the next velocity will also need to be determined in a similar fashion. Below are the equations to determine the updated position of the damped spring:

$$x_{t+1} = x_t + \frac{h}{6}(k_{1x} + 2k_{2x} + 2k_{3x} + k_{4x}) \tag{12}$$

$$k_{1x} = f_1(t, x, v) \tag{13}$$

$$k_{2x} = f_1(t + \frac{h}{2}, x + \frac{hk_{1x}}{2}, v + \frac{hk_{1v}}{2}) \tag{14}$$

$$k_{3x} = f_1(t + \frac{h}{2}, x + \frac{hk_{2x}}{2}, v + \frac{hk_{2v}}{2}) \tag{15}$$

$$k_{4x} = f_1(t + h, x + hk_{3x}, v + hk_{3v}) \tag{16}$$

Likewise, the following equations are used to determine the updated velocity of the damped spring system:

$$v_{t+1} = v_t + \frac{h}{6}(k_{1v} + 2k_{2v} + 2k_{3v} + k_{1v}) \tag{17}$$

$$k_{1v} = f_2(t, x, v) \tag{18}$$

$$k_{2v} = f_2(t + \frac{h}{2}, x + \frac{hk_{1x}}{2}, v + \frac{hk_{1v}}{2}) \tag{19}$$

$$k_{3v} = f_3(t + \frac{h}{2}, x + \frac{hk_{2x}}{2}, v + \frac{hk_{2v}}{2}) \tag{20}$$

$$k_{4v} = f_2(t + h, x + hk_{3x}, v + hk_{3v}) \tag{21}$$

In both sets of equations, $f_1(t, x, v)$ returns the current $\frac{dx}{dt}$, i.e velocity, and $f_2(t, x, v)$ returns the current $\frac{dv}{dt}$, i.e acceleration, to update the position and velocity respectively. In Figure 2 this solution can be seen plotted against the

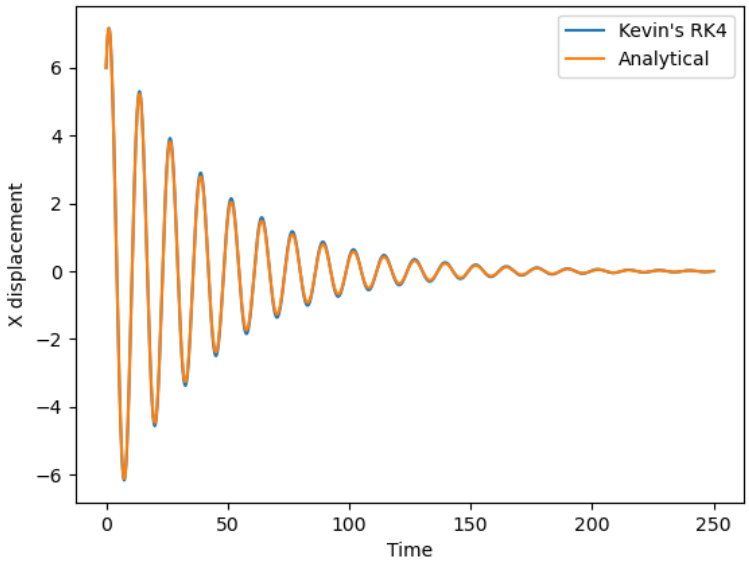

Figure 2: Plot comparing the custom RK4 solution and the analytical solution for a system with mass of 20kg, spring with force constant of 5N/m, damping constant of 1 Ns/m, initial displacement of 6m, initial velocity of 2m/s and time step of 0.05s

analytically determined solution described previously. When comparing the two of them they are nearly identical and both follow the expected behavior for an under damped spring. However, it is possible to notice that the custom

RK4 solution deviates from the analytical solution slightly by having higher displacements initially but does eventually reach the equilibrium position in the same manner.

2.1.3 Midpoint Riemann Sum

The first integration technique tested for the 1D-PIAB was the midpoint Riemann sum to determine the area of the probability density function which represents the probability of finding the particle within the bounds of the sum. This technique can be written as the following

$$Area = \sum_{n=1}^{N} f(m_i)\Delta x \tag{22}$$

$$\Delta x = \frac{b-a}{N} \tag{23}$$

where N is the total number of sub-intervals to break up the region you are integrating over and b and a are your ending and starting points respectively. In this case the function is evaluated at the midpoint of every step so as to better estimate the value of the area.

2.1.4 Trapezoidal Rule

The second integration technique tested for the 1D-PIAB was the trapezoidal rule. This rule can then be expressed using the following equation

$$Area = \sum_{n=1}^{N} \frac{f(x_n) + f(x_{n+1})}{2}\Delta x \tag{24}$$

In this case, N is still the total number of sub-intervals to break up the region of integration into and the step size, Δx is defined in the same way as in the midpoint rule. The trapezoidal rule does a better job at estimating the area under the curve than the midpoint rule by taking an average of both of the values and not looking soley at the middle of the region which you are stepping over.

2.1.5 Simpson's Rule

Lastly Simpson's rule or Simpson's composite 1/3 rule determines the area under the curve according to the following equation

$$Area = \frac{1}{3}\Delta x[f(x_0) + 4\sum_{n=1}^{N/2} f(x_{2n-1}) + 2\sum_{n=1}^{N/2-1} f(x_{2n}) + f(x_N)] \tag{25}$$

This integration technique samples more points than the trapezoidal rule and is great for functions that are smooth and continuous making it a great choice

Table 1: Integration Techniques Comparison

Num Steps	Midpoint Rule	Trapezoidal Rule	Simpsons Rule	Trapezoidal Scipy	Simpsons Scipy
5	1.0	1.0	0.9999999999999999	1.0	1.0
30	1.0000000000000002	1.0	1.0	1.0	1.0
60	0.9999999999999989	0.9999999999999988	0.9999999999999987	1.0	1.0
100	0.9999999999999992	0.9999999999999994	0.9999999999999993	1.0	1.0

for the probability density function. Each of these integration techniques were compared against each other as well as the scipy.integrate library's version of the trapezoidal and Simpsons rule. In Table 2 each integration method was called to determine the area of a box of length 1, energy level of 1, from 0 to 1 and using a varying number of sub-intervals of equal size. All of these methods should return a value of 1 and it does appear that they are relatively close to this expected value but there is clearly greater accuracy in the imported scipy methods.

3 Validation

3.1 Damped Spring-Mass System

3.1.1 Harmonic Oscillator(No Damping)

In the harmonic oscillator situation the spring mass system is undamped and continues to oscillate forever. The damping constant is equal to 0 for this case and the spring will oscillate from $\pm$ x, the initial position. As shown in Figure 3, Figure 4, and Figure 5. The explicit solution is the one that is the most unstable during this situation. Instead of oscillating within the bounds of $\pm x_0$ it increasingly oscillates further and further away from the equilibrium position accumulating in error. This is a clear violation of the conservation of energy that should be maintained in a harmonic spring. In the custom RK4 solution's case, the conservation of energy is better but it is still noticeable that the solution is increasing the amplitude over time meaning that there is also some error associated with this method. However at smaller time steps this error becomes almost unnoticeable but it is still present regardless. Additionally, comparing the custom RK4 solution and the scipy RK4 solution for this case provides near identical plots of displacement over time as seen in Figure 5, but the scipy's RK4 appears to have a more constant amplitude whereas the custom RK4 solution begins to noticeably deviate around 25 seconds.

3.1.2 Critically Damped

In the critically damped situation the spring mass system does not oscillate and reaches the equilibrium position quickly regardless of the initial velocity

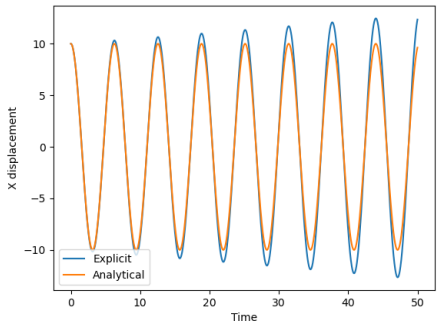

Figure 3: Plot comparing the analytical function and the explicit solution with a mass of 5kg, spring with force constant of 0N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

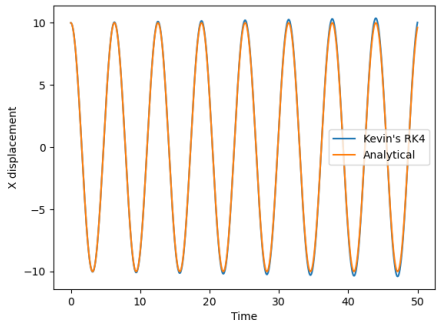

Figure 4: Plot comparing the analytical function and the custom RK4 solution with a mass of 5kg, spring with force constant of 0N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

and position. Both the explicit and custom RK4 method demonstrate this behavior as seen Figure 6 and Figure 7. While both of these solutions do differ slightly from the analytical solution, they both result in the same desired behavior for a critically damped spring. Additionally, comparing the custom RK4 solution and the scipy RK4 solution for this case provides near identical plots of displacement over time as seen in Figure 8 indicating that they both demonstrate proper behavior for tis case.

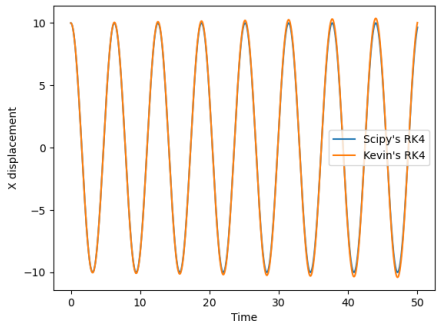

Figure 5: Plot comparing the custom RK4 solution and the scipy RK4 solution with a mass of 5kg, spring with force constant of 0N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

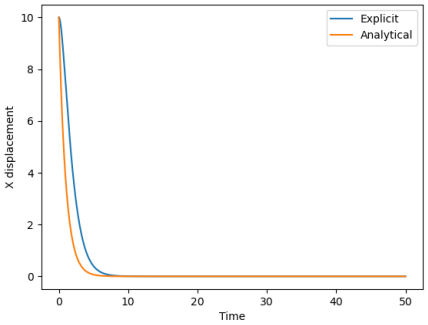

Figure 6: Plot comparing the analytical function and the explicit solution with a mass of 5kg, spring with force constant of 5N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

3.2 Probability Density of 1D-PIAB

The probability of finding the particle in specific ranges within the box was tested using different number of sub-intervals. For instance, for a region of length 1 and energy level of 1 the probability of finding the particle within 0.25 to 0.75 is 81.830988 percent. This means that the value of the integral within this region should be 0.8183099.

In this case it is clear to see that the least accurate method is the midpoint rule that only at 40 sub intervals was finally able to come close to the real

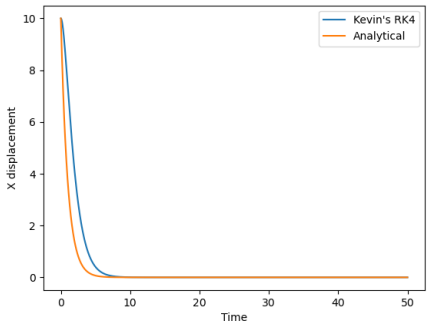

Figure 7: Plot comparing the analytical function and the custom RK4 solution with a mass of 5kg, spring with force constant of 5N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

Table 2: Integration Techniques Validation: Step Size

Num Steps	Midpoint Rule	Trapezoidal Rule	Simpsons Rule	Trapezoidal Scipy	Simpsons Scipy
5	0.8077668	0.8077683	0.7744350	0.8183098	0.8183098
10	0.7656875	0.8156875	0.8183273	0.8183098	0.8183098
20	0.7926551	0.8176551	0.8183109	0.8183098	0.8183098
40	0.8181462	0.8181462	0.8183099	0.8183098	0.8183098

answer for this integral. On the other hand, with the same number of sub-intervals Simpson's rule was able land on the analytical answer despite being more inaccurate at 5 sub-intervals. Regardless, both of the scipy library methods determined the exact answer across all runs.

4 Error Analysis

Throughout this project a variety of approximation techniques were used each with their own local and global error that is proportional to the time step in the case of the ODE problem or the sub-interval size in the case of the analytical function. Local error is the error made across one increment to another and depends on how the true value is approximated. Global error is the result of local error compounding over the course of every time/step increment. In the following sections, each method's local and global error will be derived and discussed.

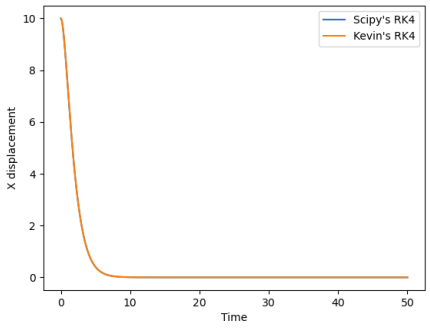

Figure 8: Plot comparing the custom RK4 solution and the scipy RK4 solution with a mass of 5kg, spring with force constant of 5N/m, damping constant of 10 Ns/m, initial displacement of 10m, initial velocity of 0m/s and time step of 0.01s

4.1 Damped Spring System

4.1.1 Error of Explicit Method

For the explicit method the value of the next position with respect to time is given by the following equation:

$$x_{t+1} = x_t + \frac{dx}{dt}dt \tag{26}$$

Assuming that the exact value of x_{t+1} is given by the Taylor expansion shown below in the following equation:

$$x_{t+1} = x_t + \frac{dx}{dt}dt + \frac{1}{2}\frac{d^2x}{dt^2}dt^2 + ... + \frac{1}{n!}\frac{d^nx}{dt^n} \tag{27}$$

then subtracting Eq.26 from Eq.27 would produce how much error there is with the explicit method, shown in the equation below:

$$Error = \frac{1}{2}\frac{d^2x}{dt^2}dt^2 + ... + \frac{1}{n!}\frac{d^nx}{dt^n} \tag{28}$$

Therefore the local error in the explicit method scales with dt^2 and this method is called a first order method. The global error of this method is then dependent on the total number of steps taken across a given interval and which is of order $O(\frac{1}{dt})$. So by taking the error of all the steps, $\frac{1}{dt}$, multipled by the error of each local step, dt^2, the overall global error $O(dt)$

4.1.2 Error of Custom RK4 Method

For the RK4 method the value of the next position with respect to time is given by the following equation:

$$x_{t+1} = x_t + \frac{h}{6}(k_{1x} + 2k_{2x} + 2k_{3x} + k_{4x}) \tag{29}$$

where each of the constants of k_{1x}, k_{2x}, etc. include compounding velocities and time steps represented by h. This means that the RK4 method takes the form of the following equation:

$$x_{t+1} = x_t + \frac{dx}{dt}h + \frac{1}{2}\frac{d^2x}{dt^2}h^2 + \frac{1}{6}\frac{d^3x}{dt^3}h^3 + \frac{1}{24}\frac{d^4x}{dt^4}h^4 \tag{30}$$

and by writing the true value of x_{t+1} as a Taylor expansion shown below:

$$x_{t+1} = x_t + \frac{dx}{dt}h + \frac{1}{2}\frac{d^2x}{dt^2}h^2 + ... + \frac{1}{n!}\frac{d^nx}{dt^n} \tag{31}$$

subtracting the two equations as show in the previous section produces error with a leading term as shown below:

$$Error = \frac{1}{120}\frac{d^5x}{dt^5}dt^5 + ... + \frac{1}{n!}\frac{d^nx}{dt^n} \tag{32}$$

Therefore the local error in the RK4 method scales with h^5 and this method is called a fourth order method, hence the 4 in RK4. The global error in this method is similar to the relationship described for the explicit method. Since the global error is dependent on the total number of time steps and has error of order $O(\frac{1}{h})$ the product of the two produces and overall global error of $O(h^4)$

4.2 Probability Density of 1D-PIAB

4.2.1 Error of Midpoint Rule

The midpoint rule approximates the value of the integral from some point, let's say x=0, to some step size, h. The true value of this integral given a function $f(x)$ is given by integrating its Taylor series as shown below:

$$\int_0^h f(x)\,dx \; = \int_0^h [f(0) + xf^{'}(0) + \frac{1}{2}x^2f^{''}(0) + \frac{1}{6}x^3f^{'''}(0)...]\,dx \tag{33}$$

which simplifies to the following equation:

$$\int_0^h f(x)\,dx \; = hf(0) + \frac{1}{2}h^2f^{'}(0) + \frac{1}{6}h^3f^{''}(0) + \frac{1}{24}h^4f^{'''}(0)... \tag{34}$$

From here the midpoint rule approximates the function $f(x)$ and can be written i terms of its Taylor series as shown below:

$$f_{mid}(x) = f(0) + \frac{1}{2}hf^{'}(0) + \frac{1}{2}\frac{1}{2}^2h^2f^{''} \tag{35}$$

the integral from this point can be calculated by multiplying by h to yield the following equation:

$$\int_0^h f_{mid}(x)\,dx \;= hf(0) + \frac{1}{2}h^2 f^{'}(0) + \frac{1}{8}h^3 f^{''}(0) \tag{36}$$

The error in the midpoint method is determined by subtracting these two from each other producing the equation below:

$$Error = \frac{1}{24}h^3 f^{''}(0) + \frac{1}{24}h^4 f^{'''}(0)... \tag{37}$$

which scales with h^3 indicating that the local error is O(h^3) and the global error in the integral is O(h^2) for reasons described in previous sections.

4.2.2 Error of Trapezoidal Rule

In the trapezoidal rule the function describing the the original function is given in the following form:

$$f_{trap}(x) = f^{'}(0)x + \frac{1}{2}hxf^{''}(0) \tag{38}$$

this can then be integrated so as to be compared with the true value of the integral from 0 to h, shown below:

$$\int_0^h f_{trap}(x)\,dx \;= hf(0) + \frac{1}{2}h^2 f^{'}(0) + \frac{1}{4}h^3 f^{''}(0) + \tag{39}$$

Subtracting these equations from each other produces the error in each step of the trapezoid method yielding the following:

$$Error = -\frac{1}{12}h^3 f^{''}(0) + \frac{1}{24}h^4 f^{'''}(0)... \tag{40}$$

This result indicates that the local error of the trapezoidal method is O(h^3) and the global error in the integral is O(h^2).

4.2.3 Error of Simpson's Rule

Lastly, in simpson's rule the function describing the original function is given in the following form as a weighted average of the midpoint and trapezoidal rules in order to minimize their errors

$$f_{simp}(x) = \frac{2}{3}f_{mid}(x) + \frac{1}{3}f_{trap}(x) \tag{41}$$

integrating this over the time step h produces the following integral

$$\int_0^h f_{simp}(x)\,dx \;= hf(0) + \frac{1}{2}h^2 f^0 + \frac{1}{6}h^3 f^{''}(0) + 0h^4 f^{'''}(0) + ... \tag{42}$$

This result can then be subtracting from the Eq. 34 and since there is no coefficient in front of the h^4 the three leading terms cancel producing a result that is O(h^5) locally indicating that the global error of the integral is O(h^4).