Analysing finite difference methods for solving ordinary differential equations

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Using the Python programming language, the dynamics of a single pendulum and a double pendulum were computationally examined to analyse different finite difference methods for solving ordinary differential equations. The fourth-order Runge-Kutta (RK4) was found to be the most suitable method considering the stability and the accuracy it can provide when solving general oscillatory problems. Subsequently, RK4 was employed to model the dynamics of a double pendulum. This yielded the understanding of the motion and the variation of the energy over time from which the dependence of the system on the initial conditions and the limitations of RK4 could be inferred.

1. Introduction

Ordinary differential equations (ODEs) are vastly common in many scientific disciplines. In most cases, however, differential equations cannot be solved analytically. Thus numerical approximations to the solution are often investigated computationally by implementing various finite difference methods (FDMs). In this analysis, it is of particular interest to study the dynamics of a simple pendulum by employing the explicit and implicit Euler, Leapfrog and fourth-order Runge-Kutta (RK4) methods. Subsequently, the stability of these FDMs were determined by examining the consistency of their output with the energy conservation law. Likewise, the dynamics of a double pendulum were modelled using RK4 and its stability was determined using the energy conservation law.

2. Theory

2.1 Single Pendulum

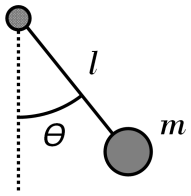

FIG. 1: Notation used for the single pendulum

The equation of a single pendulum system of mass m attached to the end of a massless rod of length l, at an angle θ to the vertical is[1]:

$$ml\frac{d^2\theta}{dt^2} = -mgsin\theta - D\frac{d\theta}{dt}, \tag{1}$$

where D is the damping coefficient and g is the gravitational acceleration. By making the small angle approximation and re-scaling all the independent variables, the dynamics of a single pendulum can be expressed by a pair of coupled first-order ODEs:

$$\frac{d}{d\hat{t}}\begin{pmatrix}\theta\\ \hat{\omega}\end{pmatrix} = \begin{pmatrix}0 & 1\\ -1 & -\hat{D}\end{pmatrix}\begin{pmatrix}\theta\\ \hat{\omega}\end{pmatrix}, \tag{2}$$

where $\hat{\omega} = \frac{d\theta}{d\hat{t}}$, $\hat{t} = \sqrt{\frac{g}{l}}t$ and $\hat{D} = \frac{1}{m\sqrt{lg}}D$.

The kinetic (T) and potential energy (U) associated with a single pendulum are given by[2]:

$$T = \frac{1}{2}ml^2\omega^2 = \frac{1}{2}mlg\hat{\omega}^2, \tag{3}$$

$$U = mgl(1-\cos\theta) \simeq \frac{1}{2}mlg\hat{\theta}^2, \tag{4}$$

where $\omega = \frac{d\theta}{dt} = \sqrt{\frac{g}{l}}\hat{\omega}$ and $(1-\cos\theta) \simeq \frac{1}{2}\theta^2$ under small angle approximation. Re-scaling Equations (3) and (4) into natural units give:

$$\hat{T} = \frac{T}{mgl} = \frac{1}{2}\hat{\omega}^2, \tag{5}$$

$$\hat{U} = \frac{U}{mgl} = \frac{1}{2}\theta^2. \tag{6}$$

Hence the sum of Equations (5) and (6) yields the total energy of the system: $\hat{E} = \hat{T} + \hat{U}$.

2.2 Double Pendulum

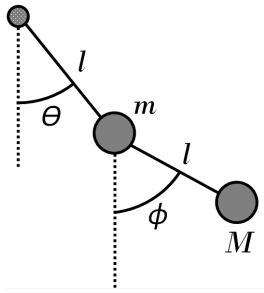

FIG. 2: Notation used for the double pendulum

Similarly, by adding a second pendulum with length l and mass M to the single pendulum mentioned in Section 2.1 at an angle ϕ to the vertical, the equations of motion for small oscillations in natural units can be expressed as a system of first-order differential equations[1]:

$$\frac{d}{dt}\begin{pmatrix}\theta\\ \phi\\ \omega\\ \nu\end{pmatrix} = \begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ -(R+1) & R & -G & 0\\ (R+1) & -(R+1) & G(1-1/R) & -G/R\end{pmatrix}\begin{pmatrix}\theta\\ \phi\\ \omega\\ \nu\end{pmatrix}, \tag{7}$$

where $\nu = \frac{d\phi}{dt}$, $R = \frac{M}{m}$ and $G = \frac{D}{m\sqrt{gl}}$ etc.

Note: the $\hat{hat}$ notation for scaled quantities are omitted in Equation (7).

The kinetic (T) and potential energy (U) associated with the double pendulum are expressed as[2]:

$$T = \frac{1}{2}Ml^2[(\omega\cos\theta + \nu\cos\phi)^2 + (\omega\sin\theta + \nu\sin\phi)^2] + \frac{1}{2}ml^2w^2, \tag{8}$$

$$U = mgl(2 - \cos\theta) + Mgl(2 - cos\theta - cos\phi). \tag{9}$$

Under small angle approximation, re-scaling into natural units and ignoring terms that are small ($\sim \theta^4$), Equations (8) and (9) can be written as:

$$\hat{T} = \frac{T}{mgl} = \frac{1}{2}((1+R)\hat{\omega}^2 + R\hat{\nu}^2 + 2R\hat{\omega}\hat{\nu}), \tag{10}$$

$$\hat{U} = \frac{U}{mgl} = 1 + \frac{1}{2}\theta^2 + \frac{1}{2}R(\theta^2 + \phi^2), \tag{11}$$

where $\nu = \sqrt{\frac{g}{l}}\hat{\nu}$ and the other symbols are as defined in Section 2.1. Hence the total energy of the system is given by the sum of Equations (10) and (11): $\hat{E} = \hat{T} + \hat{U}$. When implementing the energy conservation law in the computation, any constant was regarded as an offset and hence it was omitted.

3. Method

3.1 Finite difference methods (FDMs)

The coupled first-order ODEs for the single pendulum (Equation (2)) was computationally solved by implementing four different FDMs, namely the explicit and implicit Euler, Leapfrog and Runge-Kutta 4 (RK4) methods. For the double pendulum, RK4 method was employed to analyse its dynamics.

Explicit and Implicit Euler

Explicit Euler method approaches the integration of an ODE by utilising the Taylor expansion for the forward difference. With time $\hat{t}$ as the independent variable, Equation (2) can be written as:

$$\hat{\omega}_{n+1} = \hat{\omega}_n + (-\hat{D}\hat{\omega}_n - \theta_n)h, \tag{12}$$

$$\theta_{n+1} = \theta_n + \hat{\omega}_n h, \tag{13}$$

where h is the finite step used to calculate the values at $t + h$ up to $\mathcal{O}(h^2)$ accuracy. By solving Equations (12) and (13) iteratively, solution to the ODEs can be approximated but with a truncation (local) error incurred in dropping the $\mathcal{O}(h^2)$ terms during the derivation, leading to a global error of $\mathcal{O}(h)$.

Implicit method approaches the solution by evaluating a function $f(y)$ using an unknown value y_{n+1}. In general, for a coupled, linear first-order ODEs this is written as[3]:

$$\overrightarrow{y}_{n+1} = \overrightarrow{y}_n + h\mathbf{L}\cdot\overrightarrow{y}_{n+1}, \tag{14}$$

$$\overrightarrow{y}_{n+1} = (\mathbf{I} - h\mathbf{L})^{-1}\cdot\overrightarrow{y}_n = \mathbf{T}\cdot\overrightarrow{y}_n, \tag{15}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{L}$ is the same matrix operator as in Equation (2) and $\mathbf{T}$ is the updated matrix for the implicit Euler, which must be non-singular. Hence, for the single pendulum the corresponding equations are:

$$\hat{\omega}_{n+1} = \frac{1}{1 + h\hat{D} + h^2}[-h\theta_n + \hat{\omega}_n], \tag{16}$$

$$\theta_{n+1} = \frac{1}{1 + h\hat{D} + h^2}[(1 + h\hat{D})\theta_n + \hat{\omega}_n h]. \tag{17}$$

Again, implicit Euler has a global accuracy of $\mathcal{O}(h)$; it is a first-order method. Nevertheless, it is unconditionally stable and thus there is no critical step size h above which instability occurs. In particular, the stability analysis[3] illustrates that for a decaying problem, the solution will be stable for any positive h.

Leapfrog

The Leapfrog algorithm uses the central difference scheme to approximate the derivative between values at $n-1$ and $n+1$. This is a second-order method, leading to global error of $\mathcal{O}(h^2)$. Using the Leapfrog method for the single pendulum yields:

$$\hat{\omega}_{n+1} = \hat{\omega}_{n-1} + 2(-\hat{D}\hat{\omega}_n - \theta_n)h, \tag{18}$$

$$\theta_{n+1} = \theta_{n-1} + 2\hat{\omega}_n h. \tag{19}$$

In the computation, the first iteration for both equations are carried out using the explicit Euler method to estimate the next initial condition, improving the accuracy. In general, Leapfrog is stable for oscillating and growing solutions; but unstable for decaying solutions[3].

RK4

The Runge-Kutta methods are explicit, single-step methods which uses more than one term in the Taylor series expansion of, say, y_{n+1}. The method uses m estimations of the weighted gradient at various point in the interval $x_n \le x \le x_{n+1}$ in order to calculate the change in y. For RK4, $m = 4$ and this equates to fourth-order Taylor expansion with a local error of $\mathcal{O}(h^5)$ and a global accuracy of $\mathcal{O}(h^4)$. The general expression for RK4 is[3]:

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4), \tag{20a}$$

$$k_1 = hf(y_n), \tag{20b}$$

$$k_2 = hf(y_n + \frac{1}{2}k_1) \tag{20c}$$

$$k_3 = hf(y_n + \frac{1}{2}k_2), \tag{20d}$$

$$k_4 = hf(y_n + k_3), \tag{20e}$$

where for the single pendulum y is either θ or $\hat{\omega}$, and for the double pendulum it also refers to ϕ and $\hat{\nu}$. RK4 requires four evaluations per step; however, it was employed to analyse the dynamics of the double pendulum due to its stability and accuracy at larger values of h.

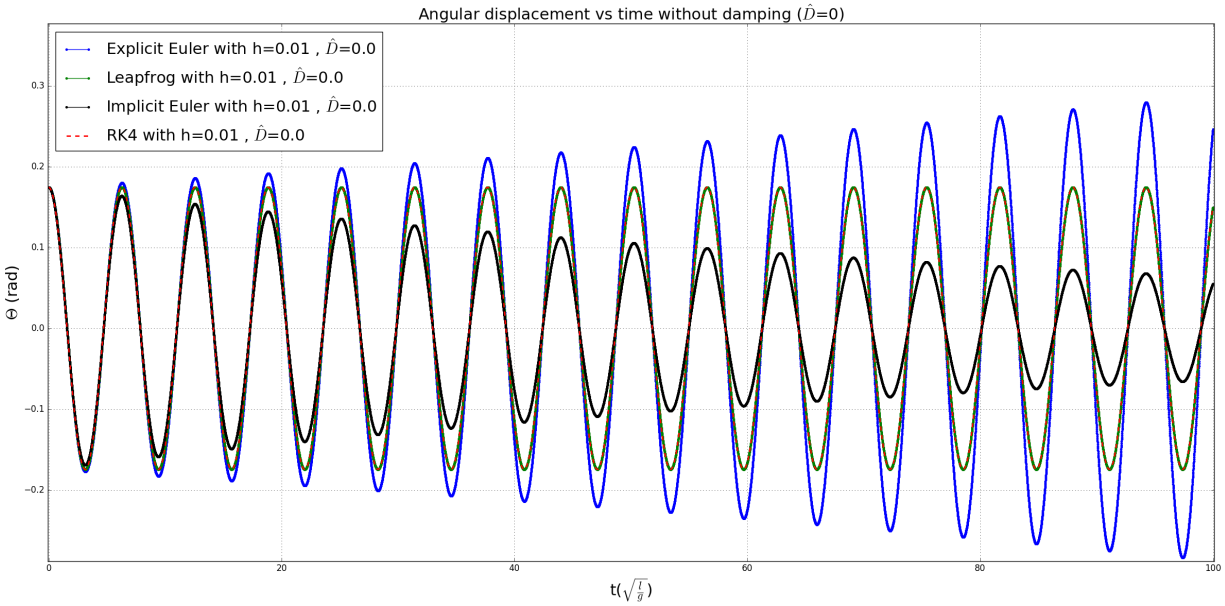

FIG. 3: Dynamics of an undamped single pendulum with $\theta_o = 10°$, $\omega = 0$ and parameters: $h = 0.01; \hat{D} = 0; 0 \leq t \leq 100\sqrt{\frac{l}{g}}$. The oscillations predicted by Leapfrog and RK4 are periodic with relatively constant amplitude. In contrast, the oscillations are becoming unbound over time for explicit Euler whereas it appears to be converging for implicit Euler.

3.2 Stability test

The energy conservation law states that the total energy of an isolated system remains constant; that is to say it is conserved over time. This is because energy can neither be created nor destroyed but transforms from one form to another. Therefore, to determine the stability of each FDMs, the variation of the total energy $\hat{E}$ with time $\hat{t}$ was examined. A FDM was concluded to be unstable when $\hat{E}$ increased with $\hat{t}$ as errors accumulated between iterations. If $\hat{E}$ either decreased or stayed relatively constant, the FDM was concluded to be stable.

The accuracy of each method was investigated by examining the change of $\hat{E}$ over $\hat{t}$ and considering whether it was consistent with the physical system described by the ODEs. For the case where the damping coefficient was zero, FDMs were concluded to be inaccurate if $\hat{E}$ deviated significantly from the initial $\hat{E}$. For a damped system, a FDM was concluded to be inaccurate when $\hat{E}$ either increased or stayed relatively constant over time. These criteria were likewise true for the double pendulum. In addition, the explicit Euler method was tested using an arbitrary amplitude oscillations by reverting the restoring force to $-mg\sin\theta$ with $\hat{D} = 0.2$ and $\theta_o \sim \frac{3}{4}\pi$. The outcome was compared with those obtained using the small angle approximation.

The critical step size h_c for each method was estimated by plotting $\hat{E}$ against step size h. In this analysis, a tolerance level of $\pm 10\%$ of the initial $\hat{E}$ was given and h_c was defined to be the step size at which the total energy of the system starts to deviate beyond this tolerance level for a given $\hat{t}$. Subsequently, by comparing the values of h_c, it was possible to determine the FDM which is most suitable for modelling the system of a double pendulum. This was taken further by implementing the bisection search method to calculate the value of h where FDMs were both relatively stable and accurate using the same range of $\hat{t}$ and the tolerance level. This was in order to make comparison with h_c and validate the accuracy of the results.

Similarly for the double pendulum, the variation of $\hat{E}$ with $\hat{t}$ was examined for $R = \{0.01, 1, 100\}$ for $G = \{0, 1\}$, and the variation of $\hat{E}$ with h was investigated in order to estimated h_c. Following this, the analysis carried out for the single pendulum was adopted.

Note: the analyses was carried out in natural units and thus the SI unit of the variables in the plots are expressed in terms of the scaling factors mentioned in Section 2.

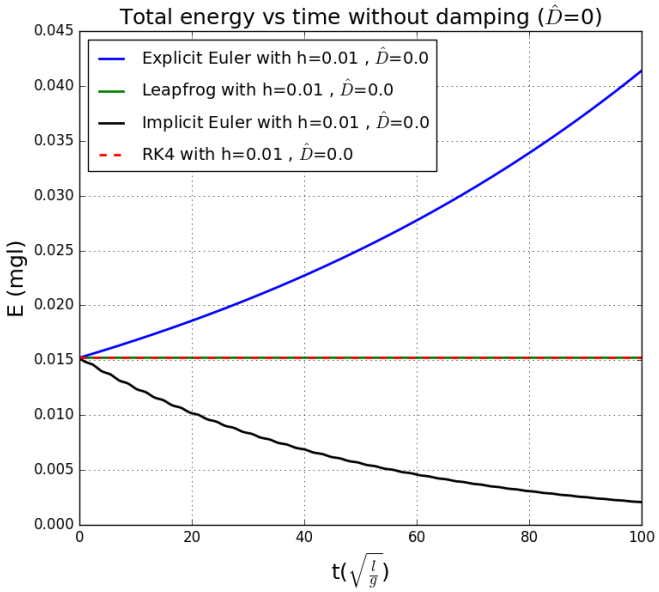

FIG. 4: The change in the total energy over time for an undamped single pendulum using the same parameters as in FIG. 3. Without damping, the law of energy conservation states that the total energy should be constant. However, the total energy is increasing and decreasing for explicit and implicit Euler, respectively.

4. Results and Discussions

4.1 Single Pendulum

The dynamics of a single pendulum without damping and its corresponding energy plot is shown in FIGS. 3 and 4.

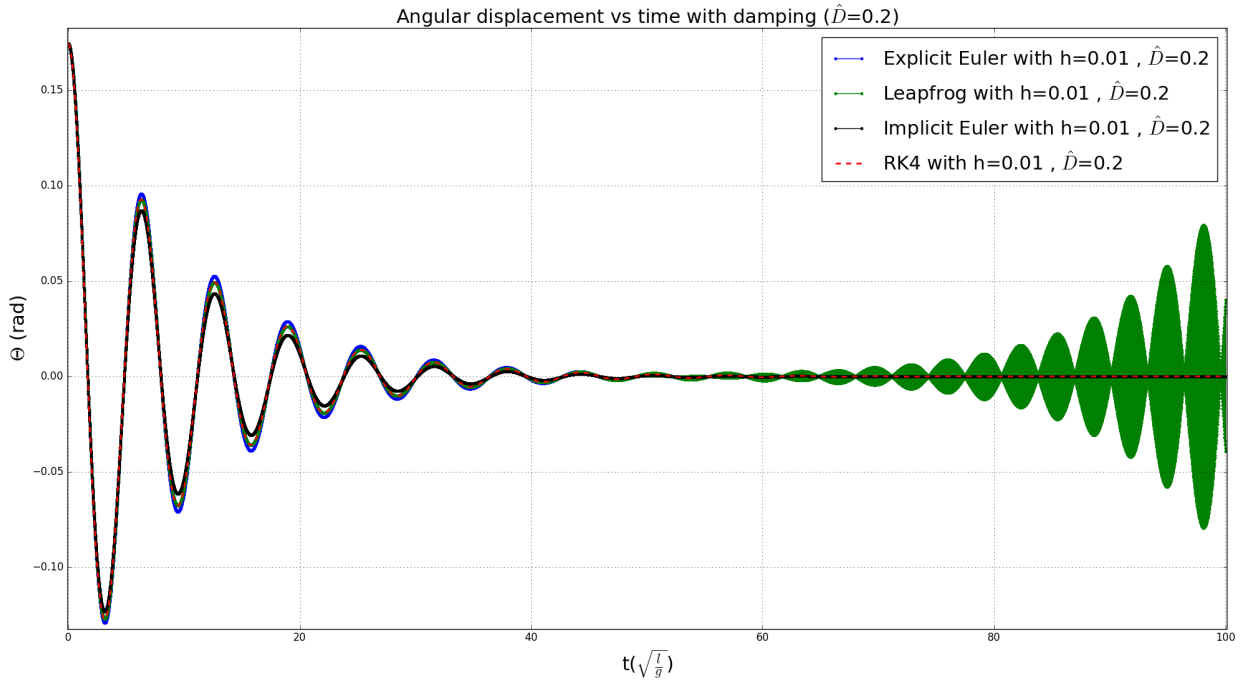

FIG. 5: Dynamics of a damped single pendulum with $\theta_o = 10°$, $\omega = 0$ and parameters: $h = 0.01; \hat{D} = 0.2; 0 \leq t \leq 100\sqrt{\frac{l}{g}}$. The oscillations predicted by RK4, and explicit and implicit Euler are converging with time. The oscillations modelled by the Leapfrog method appears to converge initially; however, it becomes unbound at higher t.

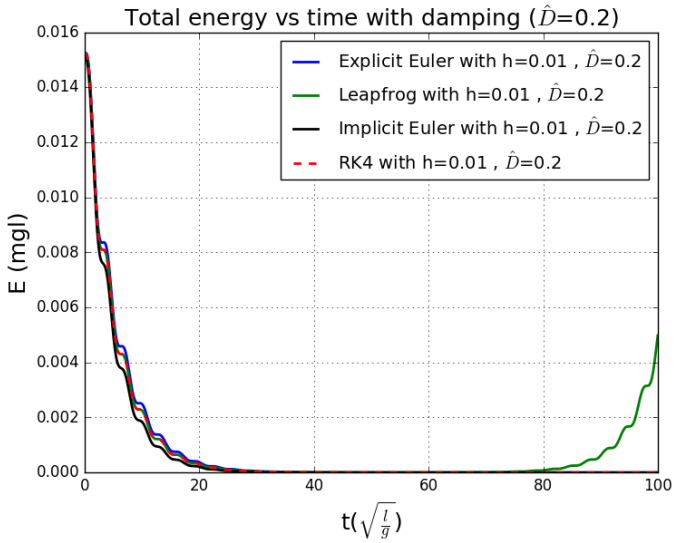

FIG. 6: The change in the total energy over time for a damped single pendulum using the same parameters as in FIG. 5. With damping, the law of energy conservation states that the total energy of the pendulum should decrease. This is true for the FDMs except Leapfrog, where the total energy is decreasing at the beginning but increases at higher t.

FIGs. 3 and 4 imply explicit and implicit Euler are inconsistent with the physical system in the undamped case as the amplitude of the oscillation are varying with time. According to FIG. 4, explicit Euler is unstable as the total energy is increasing with t. The other FDMs appear to be stable but since the implicit Euler method is unconditionally stable (Section 2.1) with a global accuracy of $\mathcal{O}(h)$, it does not seem to be an ideal method in terms of accuracy.

For the damped case, all the FDMs except the Leapfrog appear to be stable (FIG. 6). The oscillations modelled using Leapfrog seems to increase at high t and the result depicts an increase in the total energy over time. These are both inconsistent with the physical system and hence the Leapfrog method can be concluded to be unsuitable for the damped case.

Furthermore, the step size h was varied to examine the behaviour of the model and the corresponding change in the total energy when $\hat{D} = \{0.0, 0.2\}$. TABLE I summarises the results.

TABLE I: Results of the stability test for different values of h for systems with $\hat{D} = \{0.0, 0.2\}$.
Key: U - unstable; S - stable

$\hat{D}$	**FDM**	h			
		0.1	0.01	0.001	0.0001
0.0	Explicit Euler	U	U	U	U
	Implicit Euler	S	S	S	S
	Leapfrog	S	S	S	S
	RK4	S	S	S	S
0.2	Explicit Euler*	S	S	S	S
	Implicit Euler	S	S	S	S
	Leapfrog**	U	U	U	U
	RK4	S	S	S	S

*Explicit Euler became unstable when $h > 0.2$.
**The increase in E can be observed when $0 \leq t \leq 200$.

TABLE I indicates explicit Euler is unstable for all h when $\hat{D} = 0$; whereas the other FDMs yielded converging results. When $\hat{D} = 0.2$, however, Leapfrog yielded a diverging result for all h values stated. Implicit and RK4 are the only two FDMs that appeared stable for both systems. Interestingly, explicit Euler became unstable, yielding unbound oscillations when $h > 0.2$. This is consistent with the theory. By writing Equations (12) and (13) in matrix form and applying the stability con-

dition on the eigenvalue λ of the update matrix for the under-damped case yields:

$$|\lambda_{\pm}| \leq 1, \tag{21}$$

$$\lambda_{\pm} = \frac{2 - h\hat{D} \pm h\sqrt{\hat{D}^2 - 4}}{2}, \tag{22}$$

$$h \leq \hat{D}. \tag{23}$$

Similarly, for the implicit Euler, it can be shown that the method is unconditionally stable for any positive h for a damped system. Therefore, the results determined numerically are in close agreement with those calculated analytically.

To estimate the critical step size h_c, E was plotted against h with a tolerance level of $\pm 10\%$ of the initial E. The results are shown in TABLE II in addition to the results estimated by implementing the bisection search technique.

TABLE II: The estimation of the critical step size h_c using iterative and bisection search method. The initial h for the bisection search method was chosen such that it was greater than h_c calculated using the iterative method. This is due to the initial h corresponding to the upper limit whereas the lower limit was set to be 0.0001. In addition, the change in h was chosen to be 0.001 for the iterative method with the maximum h of 1.0.

Numerical method:	***Iterative***	***Bisection***	
FDM	h_c	Initial h	h_c
Explicit Euler	0.002	0.1	0.00166
Implicit Euler	0.002	0.1	0.00088
Leapfrog	0.325	0.5	0.25005
RK4	0.696	1.3	0.65005

The estimated values of h_c using both methods are in agreement with each other. The implication of the pattern observed in TABLE II is that the accuracy and the consistency of the model is maintained when utilising RK4 even with relatively large values of h. This is followed by Leapfrog. Hence, this justifies the use of RK4 in modelling the double pendulum. Furthermore, any discrepancy in the values of h_c estimated using different numerical technique could be due to the tolerance level. For a more accurate result, the tolerance level as well as the change in h should be smaller.

As a further investigation, the dynamics of the single pendulum using the explicit Euler method were studied by reverting the restoring force to $-mg\sin\theta$. The results is shown in FIG. 7.

FIG. 7 illustrates that without the small angle approximation there appears to be a phase shift developing as the oscillation propagates, causing the period to vary over time. The amplitude also differs; the magnitude of each peak is smaller. E decreases over t for in both cases which is consistent with the physical system and thus the stability appears to be unchanged when $h = 0.01$. Nevertheless, when $h = 0.3$ (FIG. 8), which violate Equation (23), the oscillation without the approximation maintains to

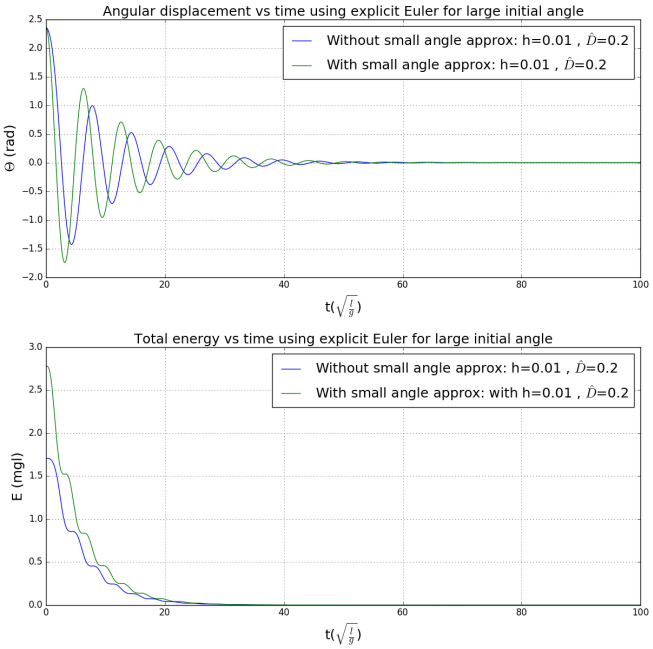

FIG. 7: The dynamics of the single pendulum and the variation of E over t with and without the small angle approximation. The parameters are: $h = 0.01$; $\hat{D} = 0.2$; $\theta_0 = \frac{3}{4}\pi$.

be stable. Therefore, it can be concluded that Equation (23) is no longer valid as the eigenvalue λ differs when reverting the restoring force to $-mg\sin\theta$, and subsequently this appears to yield a more stable result.

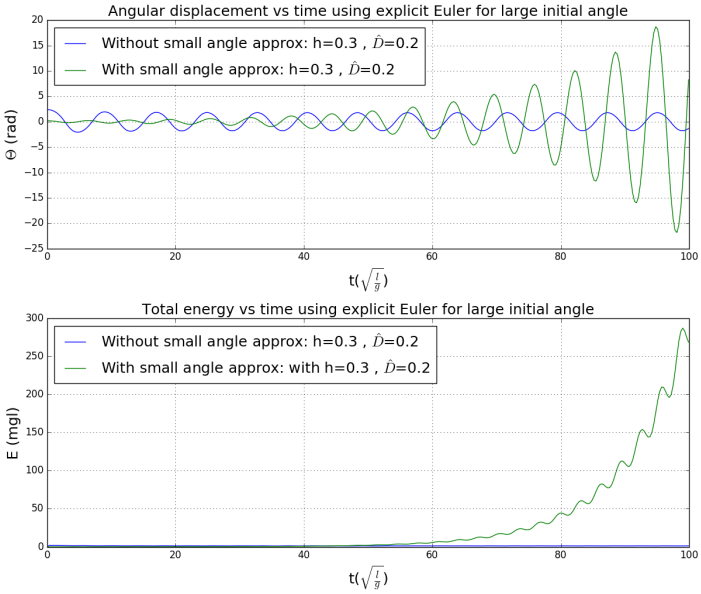

FIG. 8: The dynamics of the single pendulum and the variation of E over t with and without the small angle approximation. The parameters are: $h = 0.3$; $\hat{D} = 0.2$; $\theta_0 = \frac{3}{4}\pi$. The graph without the small angle approximation is stable; whereas the other is unstable.

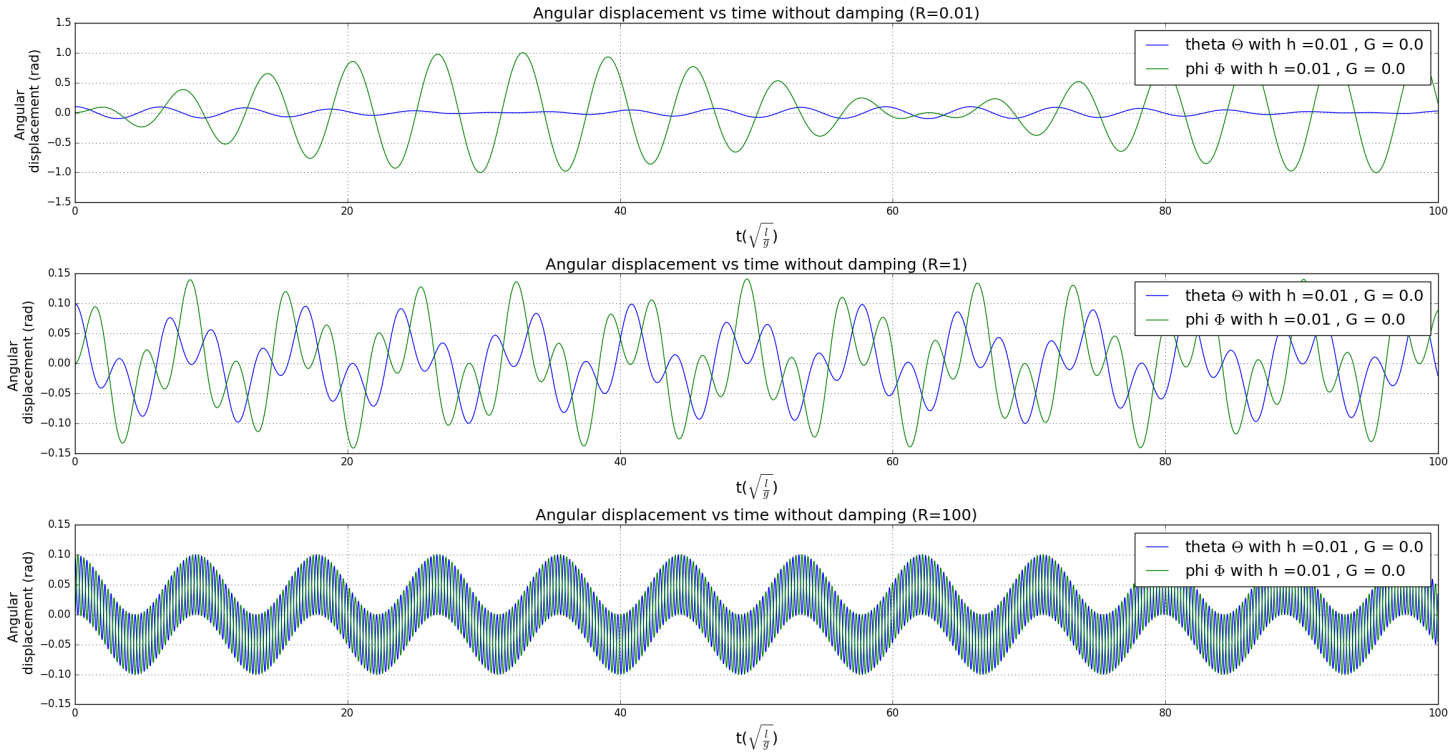

FIG. 9: The dynamics of the double pendulum with initial conditions: $\theta = 0.1$rad; $\phi = \omega = \nu = 0$ and with parameters: $h = 0.01$; $G = 0.0$; $R = \{0.01, 1, 100\}$.

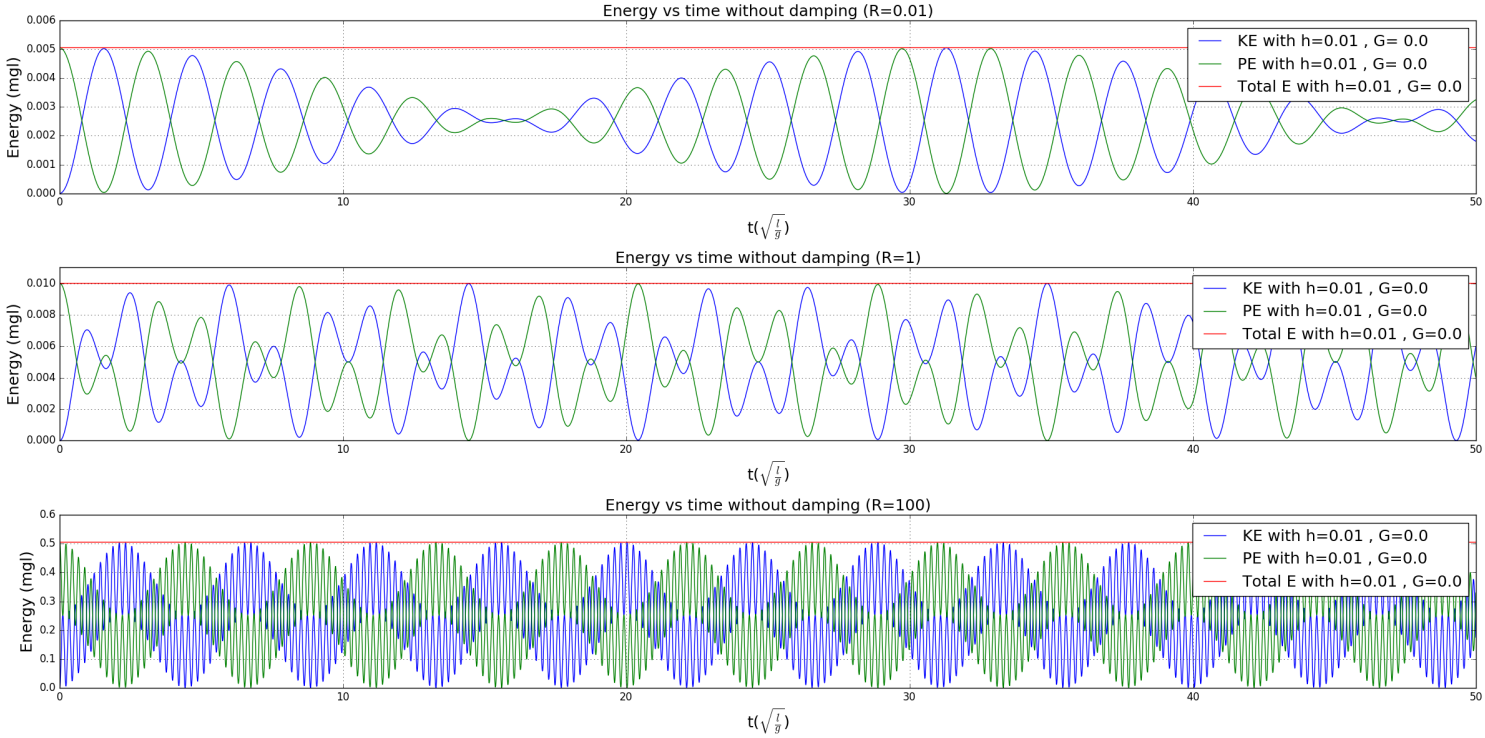

FIG. 10: The variation of E over t with initial conditions: $\theta = 0.1$rad; $\phi = \omega = \nu = 0$ and with parameters: $h = 0.01$; $G = 0.0$; $R = \{0.01, 1, 100\}$.

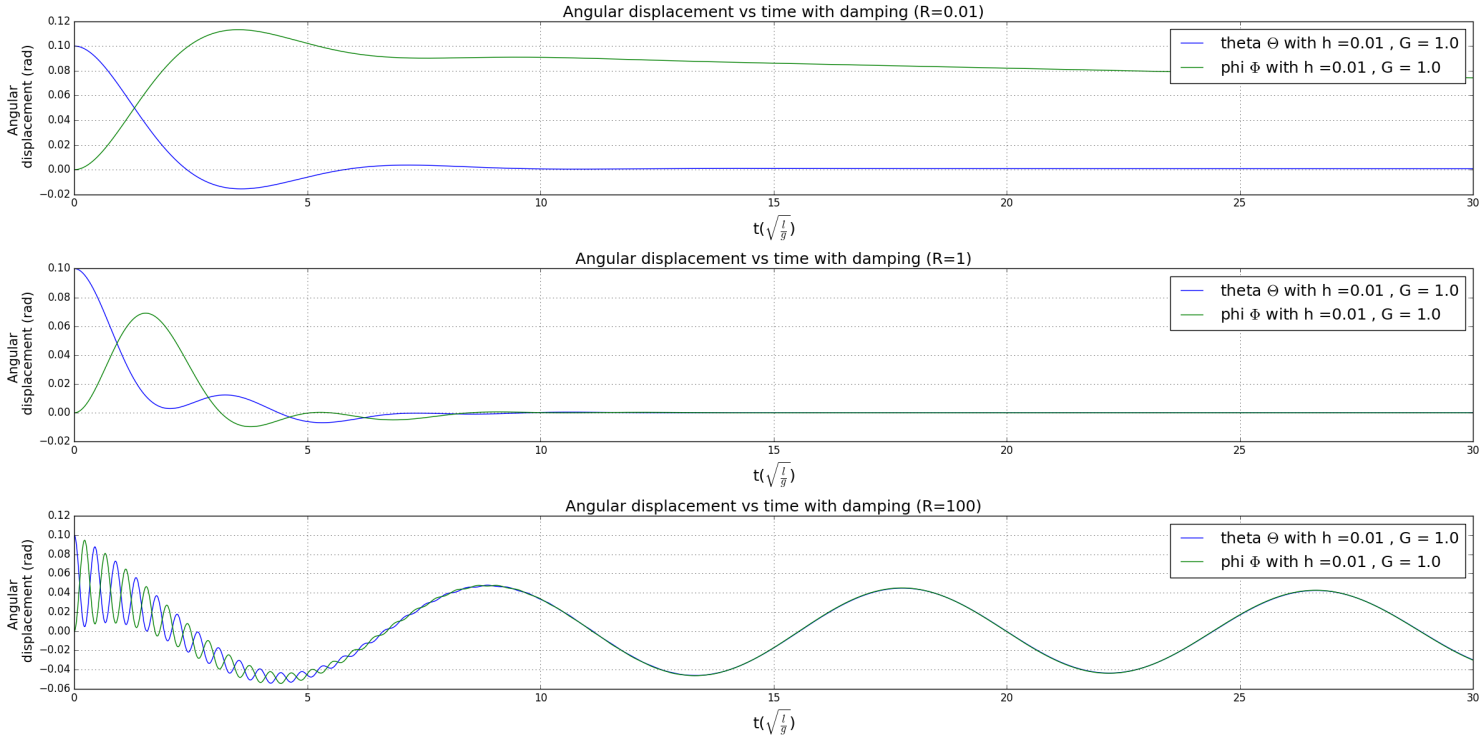

FIG. 11: The dynamics of the double pendulum with initial conditions: $\theta = 0.1$rad; $\phi = \omega = \nu = 0$ and with parameters: $h = 0.01$; $G = 1.0$; $R = \{0.01, 1, 100\}$.

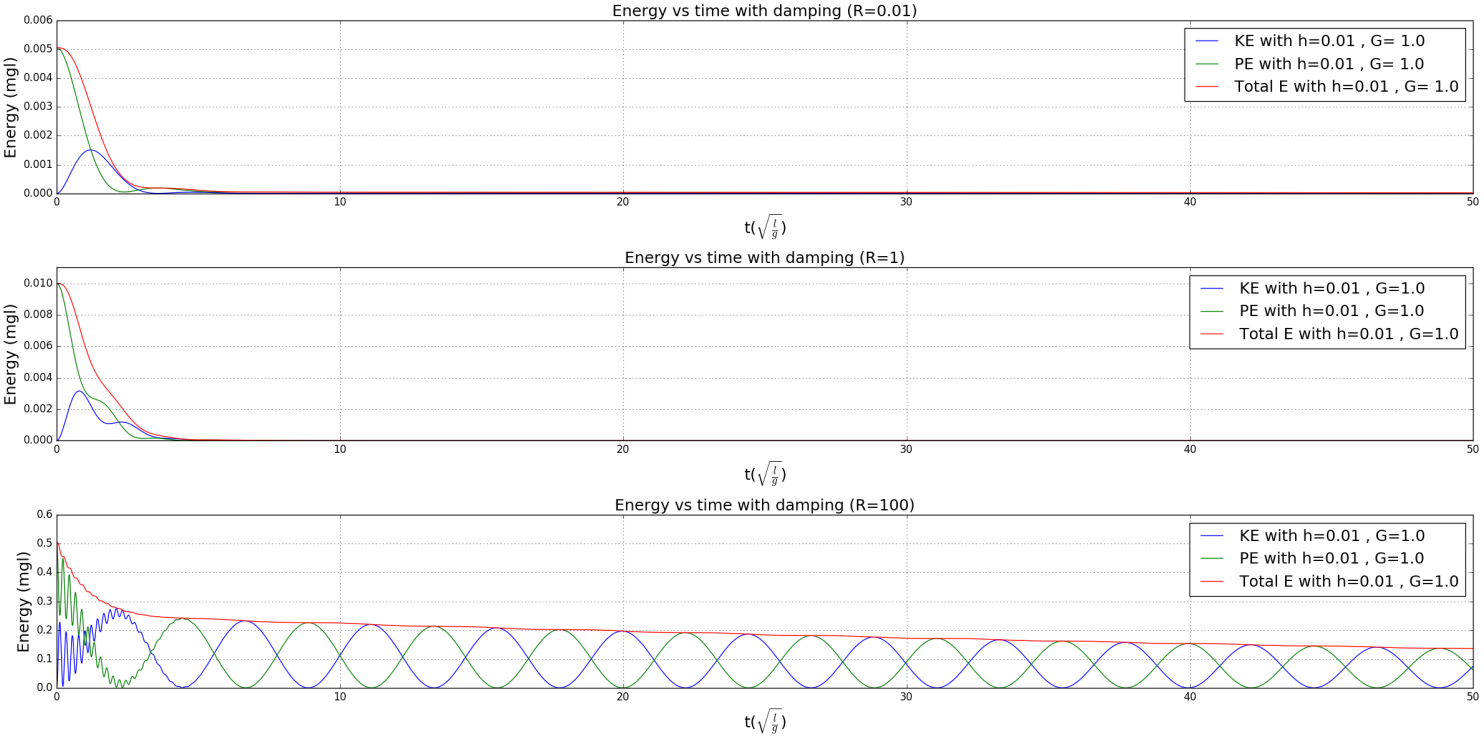

FIG. 12: The variation of E over t with initial conditions: $\theta = 0.1$rad; $\phi = \omega = \nu = 0$ and with parameters: $h = 0.01$; $G = 1.0$; $R = \{0.01, 1, 100\}$.

4.2 Double Pendulum

For the dynamics of the double pendulum, the RK4 method was employed. The results are shown in FIGS. 9 - 12. The dynamics of the double pendulum are comparatively complex. The oscillations of a simple pendulum are regular in the sense that the small deviation from the equilibrium exhibits harmonic behaviour, allowing the properties of the system to be inferred.

On the other hand, the dynamics of double pendulum exhibit sensitive dependence upon initial conditions. The regime of small oscillations for a double pendulum demonstrates the phenomenon of beating ($R = 0.01$) and displays elegant regularities otherwise (FIG. 9). This is a result of the energy being transferred cyclically between the masses. For the undamped system, the oscillations demonstrate two characteristic frequencies (normal modes). These frequencies appear to be dependent only on the ratio of the two masses R. Furthermore, the corresponding energy plot (FIG. 10) illustrates the variation of T and U over time. The total energy E is relatively constant, suggesting the model is stable. However, from the simulations, the step size h was required to be smaller for larger R. Otherwise, the oscillations for $R = 100$ with $G = 0$ exhibited a behaviour similar to that shown in FIG. 11 with damping, yielding unexpected behaviours.

When there was damping at small oscillations, the periodic behaviour described by the sum of the two harmonics no longer existed (FIG. 11). All oscillations decayed over time and the total energy also converged, indicating stability. In particular, when $R = 100$, the oscillations become synchronised and resembled the oscillations of a damped single pendulum. At relatively larger $h(= 0.1)$, the outcome was as expected when $R = \{1, 100\}$. At $R = 0.01$, however, there was a sudden increase in the oscillation and hence in the total energy. Thus the model became unstable at larger values of h.

5. Conclusion

To summarise, Runge-Kutta 4 was found to be most accurate and suitable method for modelling oscillatory motion in general. RK4 method was stable for both damped and undamped dynamics of the single pendulum. The ability to maintain its accuracy even with relatively large h was found to be far superior compared to the other FDMs. Consequently, it was utilised to model the double pendulum despite its required computation time.

RK4 was able to generate the expected results of the double pendulum. For a given h in the undamped case, however, it was found that the method was the least accurate for large values of R, yielding abnormal behaviours. Therefore, smaller h should be used for larger R. For the damped case, similar pattern was observed. An unstable outcome was found for larger values of h for $R = 0.01$. Thus, it is evident that the sensitivity of the dependence of the initial conditions increases for a more complex system.

To ensure stability of a system for general values of the parameters, the implicit Euler method could be implemented as it is unconditionally stable for any positive h for a decaying problem. But the user must keep in mind it is a first-order method with a global accuracy of $\mathcal{O}(h)$.

Further investigation could be carried out. The accuracy of the FDMs could be further analysed by calculating the differences in the oscillation periods. Since the period of a single pendulum depends only on l and g, inconsistent differences in the period could indicate the unsuitability of a method.

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[3] E. van Sebille, Y. Uchida, C. Contaldi, R. J. Kingham, *Computational Physics 2016-17 Course Note*, Department of Physics, Imperial College London, 2016, Chp.2-4