Computational Physics - Project A

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Abstract

Four finite difference methods were applied to a single pendulum system. The stability of each method was evaluated for the undamped and weakly damped cases, and the critical step size, over which the method becomes unstable, was found for each method – analytically in the case of the Euler method.

The best method was found to be RK4, and was then applied to a double pendulum system. The motion and stability of the system were analysed both in the undamped and damped cases for varying ratios of the two masses.

Single Pendulum

Aims and Methods

The stability of four numerical methods for evaluating ODEs were investigated with reference to a single pendulum system. Seeing as an unstable method eventually 'blows up', i.e. oscillates exponentially away from the true solution, the condition set for stability was that the maximum energy of the system during the run had to be less than or equal to twice the initial energy. The dimensionless energy $\widetilde{E}$ of the system was used:

$$E = T+V = \frac{1}{2}m\left(l\sqrt{\frac{g}{l}}\dot{\theta}\right)^2 + mg(l-l\cos\theta) \Rightarrow \widetilde{E} = \frac{E}{mlg} = \left(\frac{1}{2}\dot{\theta}^2+1-\cos\theta\right)$$

The maximum energy during the run, rather than the energy of the last step, was used because the energy of the leapfrog method was found to oscillate whilst remaining stable.

In the case of no damping, energy is an excellent measure because it is invariant in the system, and so any increase must necessarily be due to instability. Energy is no longer conserved in the case of damping, but it will still increase exponentially in an unstable solution. There of course remains a small error as this method accepts a relative increase in the system's energy when the system is damped.

The first thing done was to express the system in dimensionless units, and rewrite it as a matrix equation (refer to appendix A):

$$\frac{d}{d\widetilde{t}}\begin{bmatrix}\theta\\ \dot{\theta}\end{bmatrix} = \begin{bmatrix}0 & 1\\ -1 & -\widetilde{D}\end{bmatrix}\begin{bmatrix}\theta\\ \dot{\theta}\end{bmatrix}, \text{ where } \widetilde{t} = \sqrt{\frac{g}{l}}t \text{ and } \widetilde{D} = D\frac{m}{\sqrt{lg}}.$$

A run was considered to be 100 units of $\widetilde{t}$, and the number of steps evaluated for each method was adaptively changed to keep as close to this as possible. This was considered to be ample time for the method to blow up if it was unstable.

The critical step size h_{crit} was also found for each method, i.e. the step size at which the method becomes unstable. In the case of the Euler method, this can be found analytically (refer to appendix B), and is $h_{crit} = \widetilde{D}$. For the other methods, a search algorithm was implemented to find the critical step size. The algorithm was also applied to the Euler method as a control.

The value of h was found to 10 decimal places. This is not very accurate, considering the precision allowed by floats in Python, but it was felt that the level of accuracy was more than acceptable considering the inherent error in the condition used for stability.

Results

Method	h_{crit} , undamped system ($\widetilde{D}=0$)	h_{crit} , lightly damped system ($\widetilde{D}=0.2$)
Euler	0.0069326509	0.2059958039
Leapfrog	0.5518234659	Unconditionally unstable
RK4	2.8323682579	2.9541540739
Implicit Euler	Unconditionally stable	Unconditionally stable

Table 1: Critical step sizes for the 4 numerical methods

Table 1 shows the results obtained, which fit well with expectations. The Euler method has a very small h_{crit} for the undamped case, only due to the tolerance in the condition for stability. For practical purposes, it is unstable. For the lightly damped case, it fits well with the theoretical $h_{crit}=0.2$. The Leapfrog has a much larger h_{crit} for the undamped case, but is unconditionally unstable for the lightly damped case, agreeing with theory[1]. The Runge-Kutta method has an extremely large h_{crit} , for both the undamped and lightly damped systems, showing it is very resilient in its stability. The Implicit Euler method is a special case. It is unconditionally stable, i.e. there is no h_{crit} above which instability occurs[2]. However, it requires the calculation of an inverse of a matrix at each time step, making it computationally expensive.

Fig. 1 shows RK4 solutions for a lightly damped system, $\widetilde{D}=0.2$. It can be seen that even though the red solution is using an h well below the h_{crit} of approx. 2.95, it is not very accurate compared to the green solution using h = 0.1.

Hence, for a general oscillatory problem with damping, I would recommend the RK4 method, but with a smaller step size than its h_{crit} , for superior accuracy.

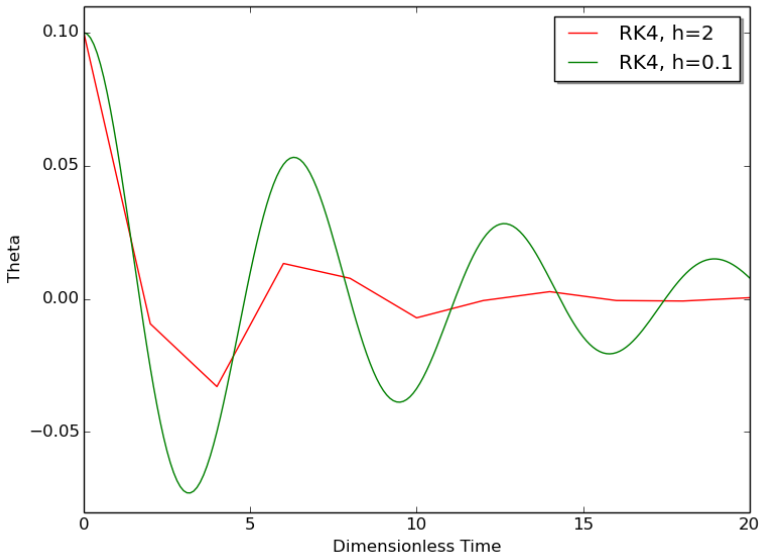

Fig. 1: RK4 solutions, varying h

Double Pendulum

Aims and Methods

The stability of a double pendulum system was investigated using the RK4 method. The same criterion for stability as the single pendulum system was used. For this system, the dimensionless energy was (see appendix C):

$$\widetilde{E}=\frac{1}{2}\left[\dot{\theta}^2+R\left(\dot{\theta}^2+\dot{\phi}^2+2\dot{\theta}\dot{\phi}\right)\right]+\left[2-\cos\theta+R\left(2-\cos\theta-\cos\phi\right)\right], \text{ where } R=\frac{M}{m}$$

A step size of 0.1 and 100 units of $\widetilde{t}$ were used initially, in accordance with the findings from the single pendulum system.

Results

The ratio R of the masses was varied while keeping the damping $G = 0$, and the energy of the system plotted. An initial step size of 0.1 was used. Fig. 2 shows the results for $R = 0.01$, and Fig. 3 shows a plot of θ and ϕ over the same timescale.

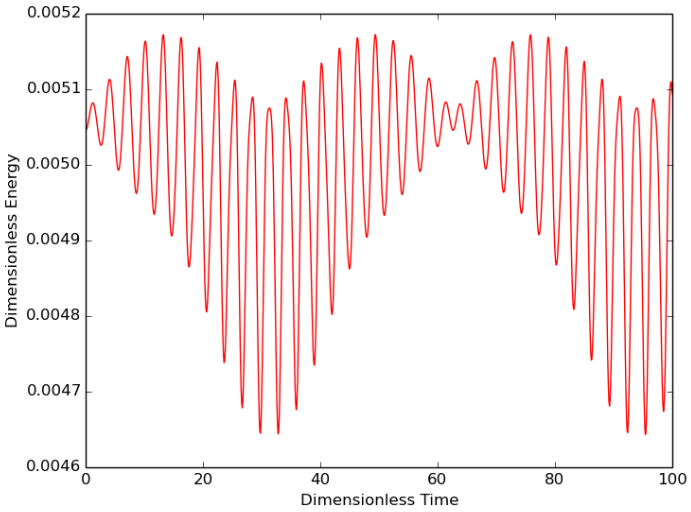

Fig. 2: Energy of double pendulum, R = 0.01

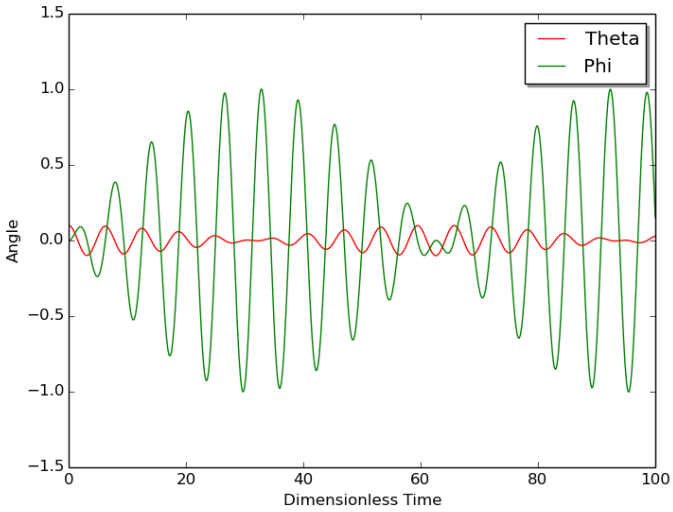

Fig. 3: Angles of double pendulum, R = 0.01

Fig. 3 shows that energy is smoothly transferred from one mass to another. It can be seen from Fig. 2 that the total energy of the double pendulum is stable, with some minor oscillations probably due to error. The large downward spikes however correspond to the shape of the amplitude of ϕ.

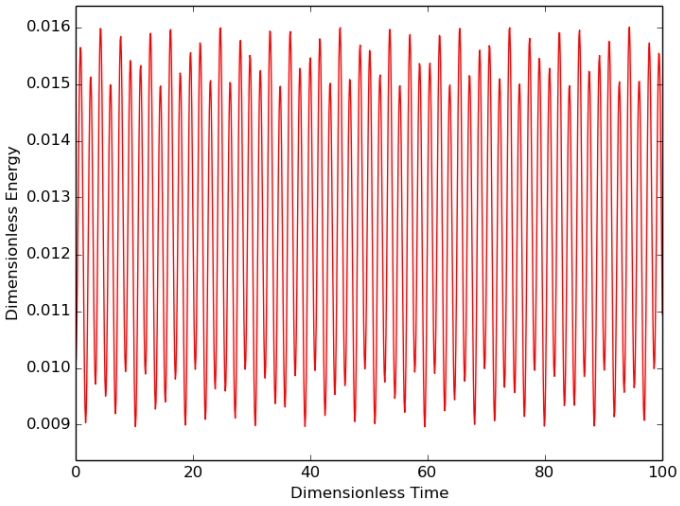

Fig. 4: Energy of double pendulum, R = 1

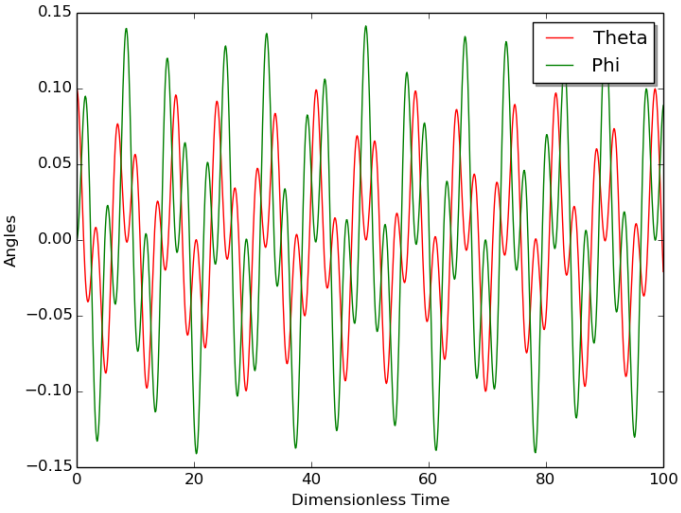

Fig. 5: Angles of double pendulum, R = 1

Fig.s 4 and 5 show the same plots, but for $R = 1$. The motion for $R = 1$ is a lot more chaotic than that of $R = 0.01$, with no clear pattern. The same goes for the energy, but it still remains stable.

Finally, the same method was applied to $R = 100$, resulting in Fig. 6. Clearly the method has not worked as well as the other two ratios, considering that the energy should remain invariant.

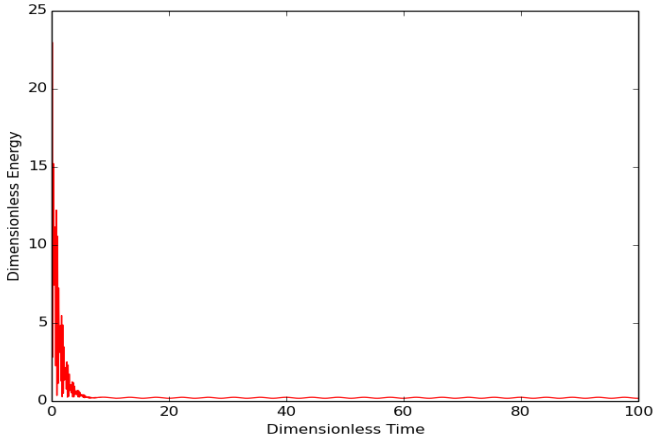

Fig. 6: Energy of double pendulum, R = 100

This might have been due to truncation error – if the motion oscillates a lot faster for $R = 1$ over $R = 0.01$, it stands to reason than the method might struggle to pick up the detail of an even denser motion. I lowered the step size by a factor of 10 to attempt to compensate for this.

Fig.s 7 and 8 show the same plots as before, for R = 100 but with a step size of 0.01. The x axis has also been zoomed in on the first 20 time units to magnify detail.

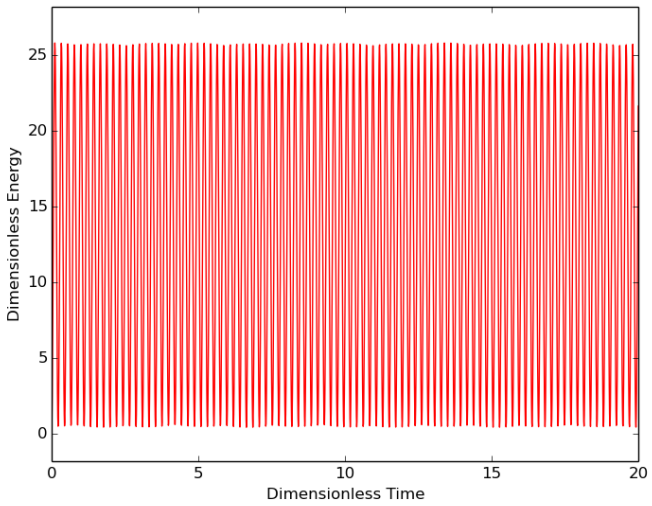

Fig. 7: Energy of double pendulum, R = 100, h = 0.01

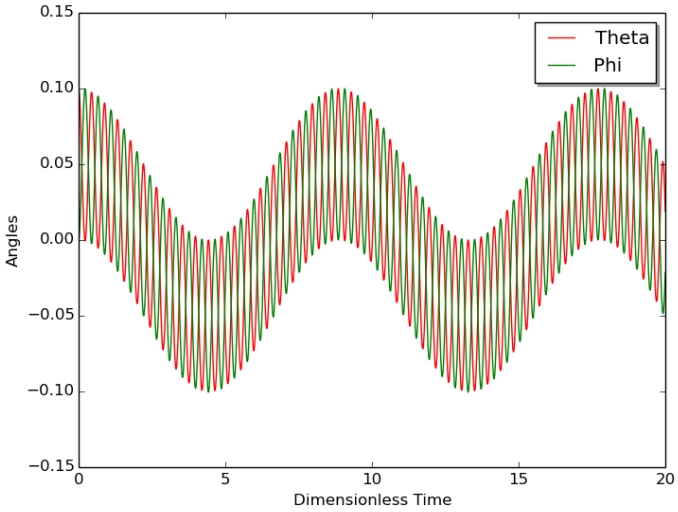

Fig. 8: Angles of double pendulum, R = 100, h = 0.01

Lowering the step size has solved the issue: the motion appears to be oscillating regularly, and the energy oscillates stably. The much heavier second mass drags the lighter mass with it, creating the overall sinusoid seen in Fig. 8.

Damping was then introduced to the system, at $G = 1$. The step size was maintained at 0.01, to ensure stability for further runs.

Fig.s 9 and 10 show the damped energy for R = 0.01 and R = 1 respectively. It can be seen that for both cases there are hardly any oscillations.

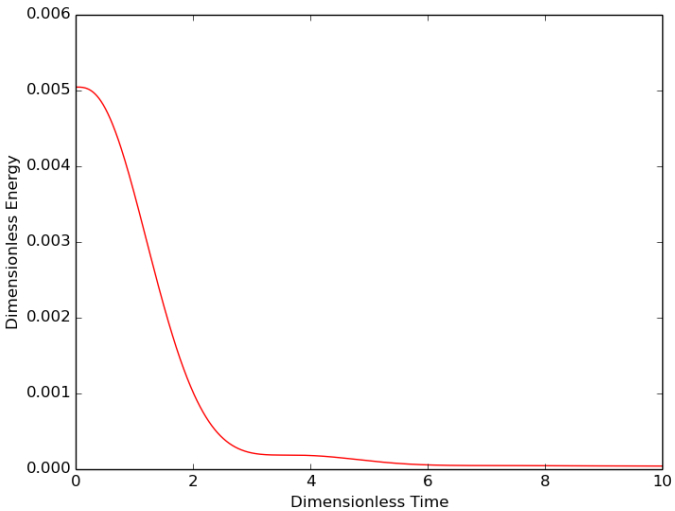

Fig. 9: Energy of double pendulum, R = 0.01, G = 1

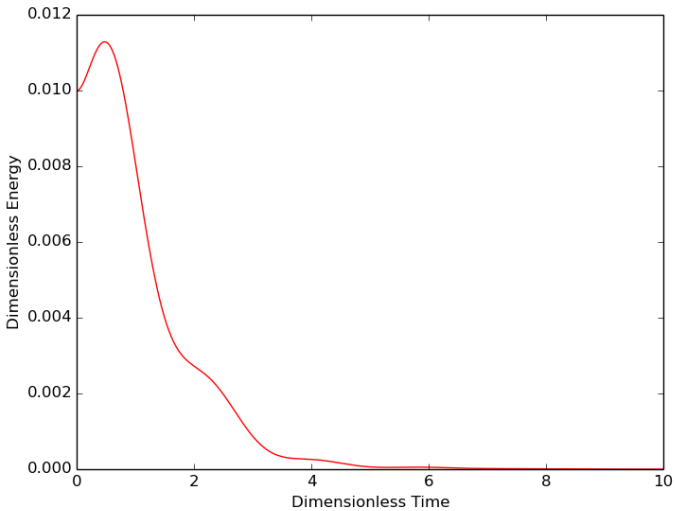

Fig. 10: Energy of double pendulum, R = 1, G = 1

Fig.s 11 and 12 show both energy and angular motion for R = 100.

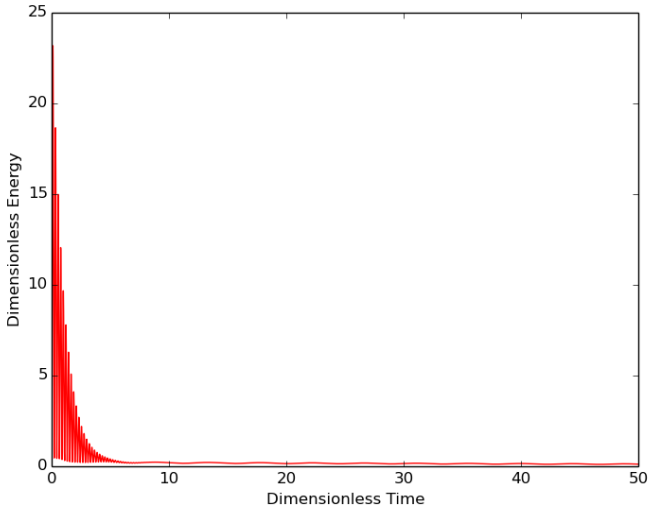

Fig. 10: Energy of double pendulum, R = 100, G = 1

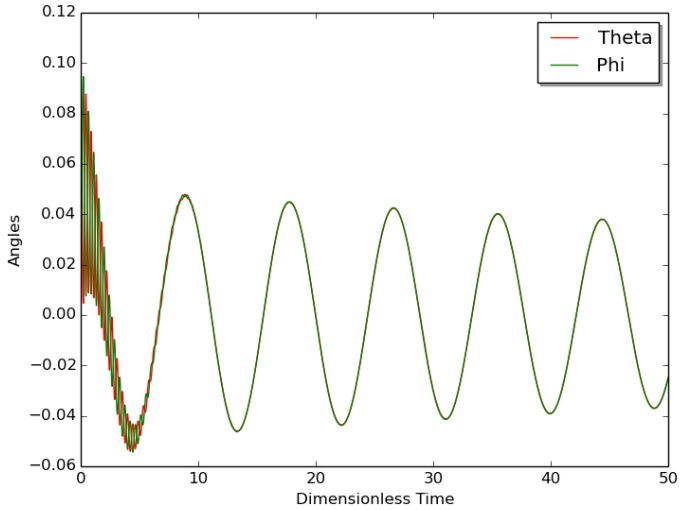

Fig. 11: Angles of double pendulum, R = 100, G = 1

This motion is a lot more interesting. The system rapidly loses energy for the first 5 or so time units, similarly to the two previous cases, but then starts to lose it much more slowly. This can be explained by looking at Fig. 11: after the first 5 time units, the angles of the two masses start coming into phase and swinging together, resisting any further energy loss. This is not visible for the two previous cases because the little energy there is in the system is damped out too quickly for the two masses to come into phase.

Conclusion

In the first part of the project, the RK4 method was judged to be the best out of the 4 due to its stability in both undamped and damped oscillation, and excellent accuracy given a small enough step size.

The RK4 method was thus used in the second part of the project, but ensuring stability was a challenge. I thought I had chosen an amply small step size of 0.1, considering the h_{crit} of over 2.5 found in the first part, and yet Fig. 6 was clearly incorrect. In order to avoid all issues relating to stability, the Implicit Euler method could have been used, which is unconditionally stable for all values of *h*. This would have been more computationally expensive, especially given the larger matrix representing the system, but perhaps would have been worth it to not have to worry about constantly changing the step size for other methods.

However, the RK4 method with the much smaller step size of 0.01 proved to be sufficiently stable and accurate to make a reasonable investigation into the dynamics of the double pendulum system.

$$Word\ count \approx 1{,}400$$

References

[1]: R. Kingham (2014), *Computational Physics*, Section 4.2, 'Multi-Step (Leapfrog) Method'
[2]: R. Kingham (2014), *Computational Physics*, Section 4.4, 'Implicit Methods'

Appendix A

The equation of motion of a simple pendulum is $ml\frac{d^2\theta}{dt^2} = -mg\sin\theta - D\frac{d\theta}{dt}$.

To make LHS dimensionless, let $\widetilde{t} = \sqrt{\frac{g}{l}}t$. This leads to $\frac{d^2\theta}{d\widetilde{t}^{\,2}} = -\sin\theta - D\frac{m}{\sqrt{lg}}\frac{d\theta}{d\widetilde{t}}$.

Let $\widetilde{D} = D\frac{m}{\sqrt{lg}}$. This leads to the dimensionless equation $\frac{d^2\theta}{d\widetilde{t}^{\,2}} = -\sin\theta - \widetilde{D}\frac{d\theta}{d\widetilde{t}}$.

In the small angle approximation $\sin\theta \approx \theta$ this equals $\frac{d^2\theta}{d\widetilde{t}^{\,2}} = -\theta - \widetilde{D}\frac{d\theta}{d\widetilde{t}}$.

This can be expressed as coupled first order ODE in matrix form: $\frac{d}{dt}\begin{bmatrix}\theta\\ \dot{\theta}\end{bmatrix} = \begin{bmatrix}0 & 1\\ -1 & -\widetilde{D}\end{bmatrix}\begin{bmatrix}\theta\\ \dot{\theta}\end{bmatrix}$.

Appendix B

The update matrix for the Euler method is $\boldsymbol{T} = \begin{pmatrix}1 & h\\ -h & 1-h\widetilde{D}\end{pmatrix}$.

For stability, the modulus of every eigenvalue of T must be less than or equal to one, i.e. $|\lambda^i| \leqslant 1$.

λ satisfy $det\left[\begin{pmatrix}\lambda-1 & -h\\ h & \lambda-1+h\widetilde{D}\end{pmatrix}\right] = 0$. Solving this gives $\lambda = \frac{2-h\widetilde{D}}{2} \pm i\frac{h\sqrt{4-\widetilde{D^2}}}{2}$.

The modulus of a complex number $a+ib = \sqrt{a^2+b^2}$, therefore for stability we require:

$|\lambda| = \sqrt{h^2 - h\widetilde{D} + 1} \leqslant 1$. Solving for h: $h(h-\widetilde{D}) \leqslant 0$.

As this is a positive quadratic, the Euler method is stable if $0 \leqslant h \leqslant \widetilde{D}$.

Appendix C

Total energy for the double pendulum system is $E_{tot} = T_m + V_m + T_M + V_M$.

$T_m = \frac{1}{2}mlg\dot{\theta}^2$. $T_M = \frac{1}{2}Mlg(\dot{\theta}+\dot{\phi})^2 = \frac{1}{2}Mlg(\dot{\theta}^2+\dot{\phi}^2+2\dot{\theta}\dot{\phi})$.

$V_m = mlg(2-\cos\theta)$. $V_M = Mlg(2-\cos\theta-\cos\phi)$.

$\widetilde{E} = \frac{E}{mlg} = \frac{1}{2}\left[\dot{\theta}^2 + R(\dot{\theta}^2+\dot{\phi}^2+2\dot{\theta}\dot{\phi})\right] + \left[2-\cos\theta + R(2-\cos\theta-\cos\phi)\right]$, where $R = \frac{M}{m}$.