Project B: Thermodynamic Simulations using the Ising Model

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Abstract

The Ising model allows to illustrate the behaviour of the spins in a ferromagnetic material with a representation of the system by a two-dimensional lattice of spins up and down. The theory predicts that the spins tend to align at low temperatures and that they pint up and down randomly at high temperature. There is thus a phase transition defined by the Curie temperature. Theses expectations are confirmed by using the Monte Carlo method. For the first part of the experiment, we only consider the internal interaction, the results are consistent with the theory. Then, a magnetic field is applied. The spins tend to align with the field when Temperature is higher than the Curie Temperature, however this effect is not very significant at a very high temperature because thermal agitation dominates. For T less than T_c, the alignment of the spins by the magnetic field is only possible if the field is strong enough.

1 Introduction

The motion of the single pendulum with mass m, length l, angle of θ to the vertical and a damping coefficient of γ is described by the second order differential equation.

$$ml\frac{d^2\theta}{dt^2} = -mg\sin\theta - \gamma\frac{d\theta}{dt} \tag{1}$$

The computation methods only work for first order ODEs, so equation (1) must be transformed into a pair of coupled ODEs. Time, t, is expressed in units of $\sqrt{\frac{l}{g}}$, where g is the gravitational constant, such that the equations are in natural units. Under the small angle approximation where $\sin\theta \approx \theta$, the coupled ODEs may be expressed as,

$$\frac{d}{dt}\begin{pmatrix}\theta\\u\end{pmatrix} = \begin{pmatrix}0 & 1\\-1 & \gamma'\end{pmatrix}\begin{pmatrix}\theta\\u\end{pmatrix} = \boldsymbol{L}.\begin{pmatrix}\theta\\u\end{pmatrix} \tag{2}$$

where $u = \frac{d\theta}{dt}$ and $\gamma' = \frac{\gamma}{m\sqrt{1/lg}}$

Discretising (2) allows the Euler method to be written as,

$$\boldsymbol{y_{n+1}} = \boldsymbol{y_n} + h\boldsymbol{L}.\boldsymbol{y_n} = \begin{pmatrix}1 & h\\-h & 1-h\gamma'\end{pmatrix}.\boldsymbol{y_n} = \boldsymbol{T}.\boldsymbol{y_n} \tag{3}$$

where $\boldsymbol{L}$ is the 2×2 differential matrix, $\boldsymbol{T}$ is the update matrix and $\boldsymbol{y}_n = \binom{\theta}{u}$

Similarly, the Leapfrog method may be written as,

$$\boldsymbol{y_{n+1}} = \boldsymbol{y_{n-1}} + 2h\boldsymbol{L}.\boldsymbol{y_n} \tag{4}$$

Finally the RK4 Method may be written as,

$$\begin{aligned}
\boldsymbol{y_{n+1}} &= \boldsymbol{y_n} + \frac{1}{6}(\boldsymbol{k_1} + 2\boldsymbol{k_2} + 2\boldsymbol{k_3} + \boldsymbol{k_4})\\
\boldsymbol{k_1} &= h\boldsymbol{L}.\begin{pmatrix}\theta_n\\u_n\end{pmatrix}\\
\boldsymbol{k_2} &= h\boldsymbol{L}.\begin{pmatrix}\theta_n + \frac{1}{2}k_1^\theta\\u_n + \frac{1}{2}k_1^u\end{pmatrix}\\
\boldsymbol{k_3} &= h\boldsymbol{L}.\begin{pmatrix}\theta_n + \frac{1}{2}k_2^\theta\\u_n + \frac{1}{2}k_2^u\end{pmatrix}\\
\boldsymbol{k_4} &= h\boldsymbol{L}.\begin{pmatrix}\theta_n + k_3^\theta\\u_n + k_3^u\end{pmatrix}
\end{aligned} \tag{5}$$

where k_1^θ is the θ component of $\boldsymbol{k_1}$ and k_1^u is the u component of $\boldsymbol{k}_1$. Using equation (3) (4) (5), we can simulate the time evolution of the single pendulum. For small angles, the equations of motion for the double pendulum are

$$\begin{aligned}
ml\frac{d^2\theta}{dt^2} &= -(m+M)g\theta + Mg\phi - \gamma\frac{d\theta}{dt}\\
Ml(\frac{d^2\theta}{dt^2} + \frac{d^2\phi}{dt^2}) &= -Mg\phi - \gamma\frac{d\theta}{dt} - \gamma\frac{d\phi}{dt}
\end{aligned} \tag{6}$$

This can be written as first order ODEs as,

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

where $R = M/m$, $G = \gamma/(m\sqrt{gl})$ and times in units of $\sqrt{l/g}$

2 Stability

The stability of the methods can be tested by checking whether the system conserved energy. The total energy of the single pendulum under the small angle approximation and in natural units is,

$$E_{Single} = \frac{1}{2}(\theta^2 + \dot{\theta}^2) \tag{8}$$

and the total energy of the double pendulum is given by,

$$E_{Double} = \frac{1}{2}(R(\dot{\theta} + \dot{\phi})^2 + \dot{\theta}^2 + (R+1)\theta^2 + R\phi^2) \tag{9}$$

The Conservation of Energy allows us to adopt a trial and error type of numerical analysis with the Leapfrog and the RK4 methods by narrowing down the range of step sizes where the energy converges or diverges. Noted that for Euler, this could be done analytically with ease.

Ideally, E should be constant throughtout the computations. If the method is unstable, the error eventually exceeds the initial values of θ and ϕ, causing the conservation of energy to be broken. This is due to the propagation of errors and the solution becomes divergent and unable to converge to a constant value.

A numerical method is written to do a trial and error algorithnm to find the optimal h. Algorithnmically, we set up h such that it is divergent over a long timescale and we could iterate the system such that the iterations stop to give a h in the case where the energy does not exceed the threshold value.

An investigation of accuracy is also done by varying h against the energy difference, δE,between $E(t = 0)$ and $E(t = t')$. This can give us the underlying relationship between the stepsize and the errors in energy. Namely, that is how errors grow with h.

2.1 Critical Stability for Euler

Using the stability analysis for the Euler update matrix T, it is possible to find an exact point where the method goes from stable to unstable at a particular h and it is known as the critical step size. For Euler, this is done by solving the eigenvalue equation for the update matrix, T. The eigenvalue λ is found to be

$$\lambda_{\pm} = 1 - \frac{\gamma' h}{2} \pm \frac{ih}{2}\sqrt{4 - \gamma'^2} \tag{10}$$

The critical step size can be found as $h = \gamma'$ for the damped case and the Euler method is unstable for all value of h in the undamped case as the critical timestep is an imaginary number.

3 Results and Discussion

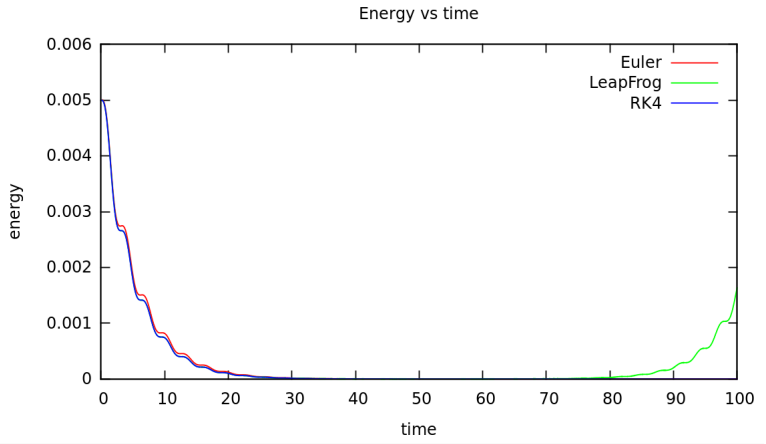

Figure 1: "Energy vs time" of Euler, Leapfrog and RK4 for a damped pendulum (The Green line shows the LF is unstable and diverging)

3.1 Single Pendulum

In general, it is expected that for $\gamma' = 0$, an oscillatory solution would be found and a decaying oscillatory solution would be found for a lightly damped pendulum($\gamma' = 0.2$). For the RK4 method, these expectations are fulfilled. However, the damped Leapfrog and undamped Euler methods are unstable for all h and the amplitude of the oscillatons exploded as well as the energy. The explosion of the amplitude is due to the Euler method having a global error of $O(h)$ and so the error increases exponentially with respect to time. On the other hand, the Leapfrog and RK4 methods are shown to be stable for the undamped pendulum. Both methods exhibited oscillatory motions with unchanging amplitude; both methods are stable at a reasonable step size.

For the damped single pendulum, Euler is shown to be stable, but the $energy - \theta$ plot shows that the energy is not conserved when compared to

Table 1: Critical Time-step for different methods: This shows RK4 is by far the more stable method

Methods	Undamped	Damped
Euler	Unstable	γ'
Leapfrog	$0.948683 \pm 1e-5$	Unstable
RK4	$2.95058 \pm 1e-5$	$2.82843 \pm 1e-5$

RK4 results. The Euler method is stable but not accurate and does not give the correct solutions for a damped single pendulum.

The Leapfrog method is unstable for the damped pendulum, breaking the conservation of energy (Shown in Figure 1 and 3). This is due to the initial Euler step at the beginning of the iteration that propagates throughtout the iterative steps and continues to diverge; the error could not converge as the solution is not a perfectly oscillatory solution.

The RK4 method is stable and accurate; it does not break the energy conservation laws. In terms of stability, table 1 shows RK4 is a factor of 2.8 more stable than others. Thus, the RK4 is chosen for the double pendulum computation.

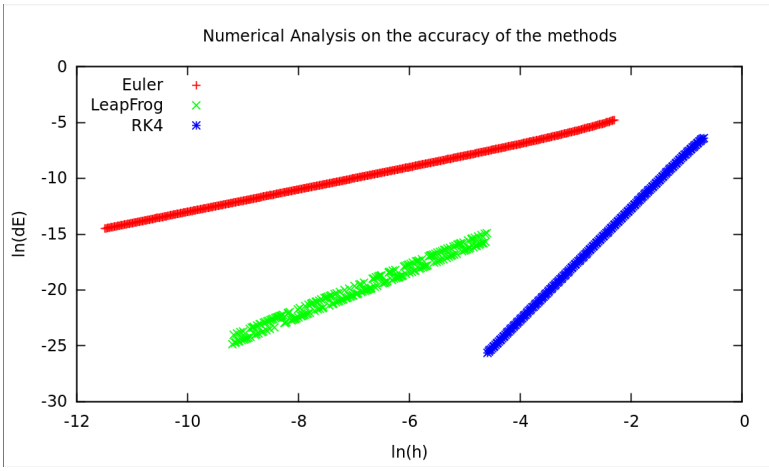

Figure 2: ln(dE) vs ln(h)(The gradient of the curve is the global accuracy of the method)

In addition, we have done a numerical analysis on the accuracy of the methods. This is done by using the energy consideration to obtain the error in energy, dE, at $t = t'$ using different timesteps. A log graph is plotted

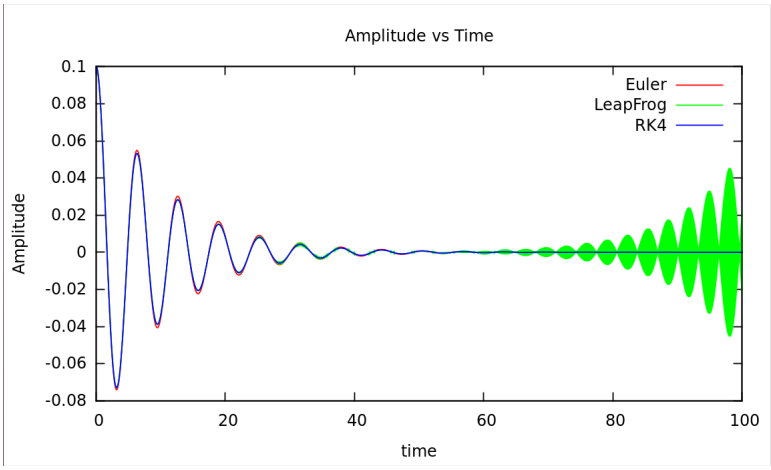

Figure 3: "Amplitude vs time" of Euler, Leapfrog and RK4 for a damped pendulum(Again, Diverging LF)

Table 2: Results on the accuracy of the method, derived numerically(c.f Figure 2)

Method	d(ln(dE))/d(ln(h))	Global accuracy error
Euler	1.029 ± 0.001	$O(h)$
Leapfrog	1.998 ± 0.019	$O(h^2)$
RK4	4.00 ± 0.05	$O(h^4)$

and the results agree with the theoretical accuracy of each method shown in table 2 and figure 2. Figure 2 shows a log plot for the error in energy as a function of step size with a constant gradient. These gradients represent the global accuracy, $O(h^n)$ of the method since $ln(O(h^n)) = n(ln(O(h))$. These values agree with the theory within errors. Again, this also shows that RK4 is a better and more superior method.

3.2 Double Pendulum

The dynamics of the double pendulum follows two normal modes of motion depending on initial conditions(Figure 4). The RK4 method is used to model the dynamics of the damped and undamped double pendulum. Again, the stability is tested with the energy consideration under three different mass ratios: $R = 0.01$, $R = 1$ and $R = 100$. By linearising the ODEs with the small angle approximation, the equations are linear and do not show

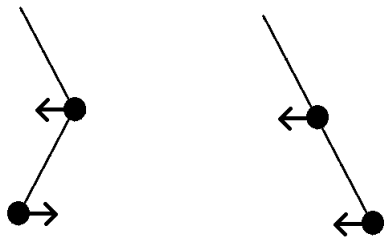

Figure 4: Normal modes for the double pendulum, G=0, R=1

chaotic behavior. In general, the solutions are shown to exhibit constant frequency. The shape of the motion depends a lot on the R and G. The general behavior is a linear superposition of two pendulums, creating a more complex structure in the oscillations. For the undamped cases where G=0, each value of R produced a diamond shape in the $\theta - \phi$ plots(Figure 5). The trajectories demonstrate how for given initial parameters, ϕ and θ are limited in amplitude to conserve energy. For all mass ratios, ϕ is maximum when $\theta = 0$. This is obvious as the first mass only begins to decelerate at this point. During the computations, we need to change the time step by more than an order of magnitude to ensure the iterations are stable, especially at extreme cases like $R = 0.01$ and $R = 100$, suggesting that the stability is sensitive to the ratio of masses.

In the case of $R = 1$, there is a $\pi/2$ phase difference between the masses. When $m >> M$, this is when the upper mass is being practically stationary, while the lower swings with its natural frequency. Figure 5 shows that, in this case, the range of ϕ is ≈ 10 times that of θ. The final case is $M >> m$. In this case, the pendulum swings like a single pendulum of length $2l$; the motion of M becomes a single pendulum as m tends to 0. And when the masses are set to swing opposite to each other, the lower mass ramins almost stationary while the upper one executes rapids oscillation.

The dynamics for the damped case, $G = 1$, are shown in figure 8 and 7. When $R = 1$, the two masses again oscillates $\approx \frac{\pi}{2}$ out of phase until the motion becomes negligible (A decaying version of the undamp case). For $M >> m$, the dynamics is similar to the undamped case with the lower mass dominating the oscillations. For $m >> M$, the damping for the lighter m takes an unusually longer time to reduce from its maximum angle and it is an unphysical result.

Again, the method is unstable for $h = 0.1$ at $R = 100$ and $R = 0.01$ in

the damped case. By using $h = 0.005$ or lower, all simulations conserved energy and remain stable.

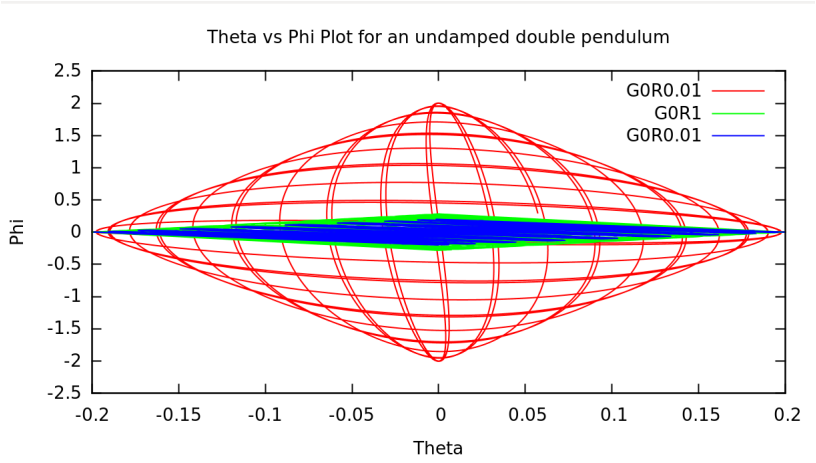

Figure 5: Θ-Φ plot for un undamped double pendulum

4 Conclusion

We have investigated how effective the three iterative methods can simulate the motion of a single and double pendulum. We have found that the Leapfrog method works well for oscillatory periodic functions but fails to work for decaying functions. Euler's method is the least accurate and least stable, especially for undamped cases. The RK4 method is found to be the most approriate for the double pendulum problem, giving both stable and accurate results for the damped or undamped cases with meaningful physical solutions. Using the energy considerations, we are able to determine effectively the stability and accuracy of each method without calculating the analytical solution.

Using the RK4 method to model the double pendulum, we test different timesteps for the damped and the undamped cases. The results remain stable for a reasonable timespan and so using the RK4 method is justified. Smaller time steps are needed for extreme cases like $R = 0.01$ and $R = 100$. We also find that the oscillations followed 2 distinct modes of behaviour depending on the initial conditions.

An interesting direction of further investigation is the comparison of the analytical results with the numerical results in understanding the nature of

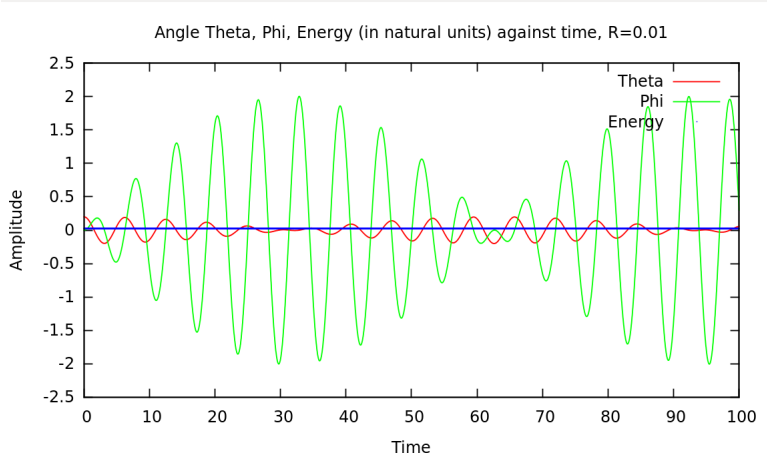

Figure 6: Theta,Phi and Energy plot, G=0,R=0.01 (This is m being stationary due to its large mass and M following large oscillations close to its natural frequency, interesting to see a transfer of energy between the pendulums; the maximum amplitude for M is at the minimum amplitude for m, vice versa)

errors behind the computation. For the damped single pendulum, the analytical value for the exponentially decaying energy can be used to understand where exactly the solutions become unstable.

Approx Words Count: 1480 (Excluding caption)

5 Reference

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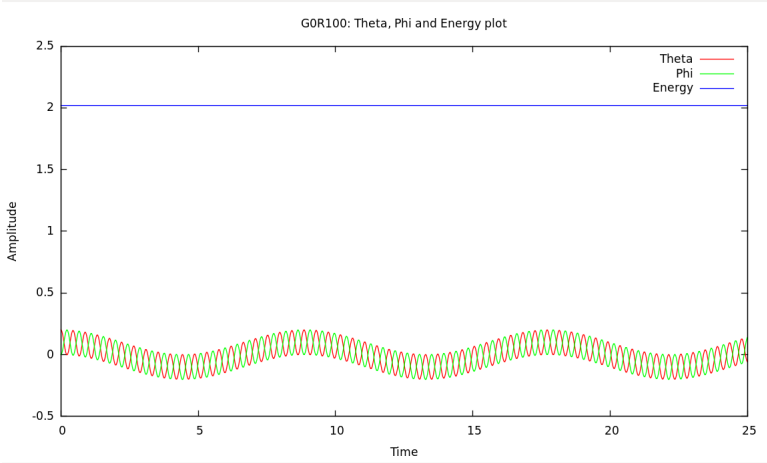

Figure 7: Theta,Phi and Energy plot, G=0,R=100 (As m gets smaller, this will tend to a single pendulum with the intermediate oscillations disappearing)

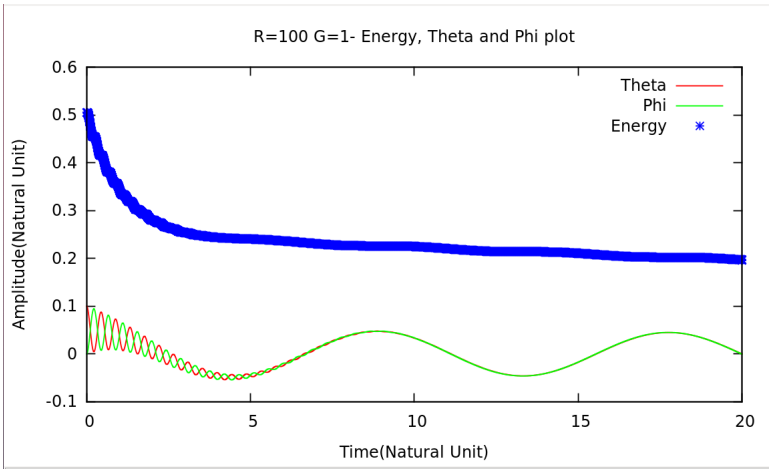

Figure 8: Theta,Phi and Energy plot, G=1,R=100 (Same dynamics as the undamped pendulums but interesting to see damping help theta and phi to converge, this make sense as the more massive lower pendulum takes a more dominant role in driving the damped oscillations)

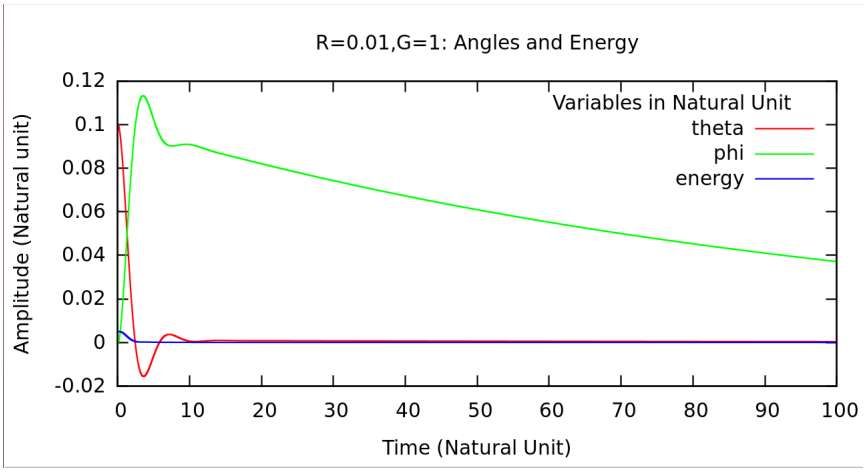

Figure 9: R=0.01,G=1:Theta, Phi and Energy plot (This is an unphysical solution with theta and energy damped to zero as normal very quickly but Phi(The lighter and lower pendulum) hanging in mid-air; this shows RK4 method is inefficient in this case.)