Homework 3: Computational Physics

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September 25^{th}, 2020

1 Problem 1

In the small angle approximation, the energy of a pendulum:

$$E_{tot} = \frac{1}{2}mL^2\omega^2(t) + \frac{1}{2}mgL\theta^2(t) - mgL$$

Analytically show that E monotonically increases with time when the Euler method is used to compute the motion.
Let's prove that the total energy E_{tot} is actually conserved in the small angle approximation. First, let's find the equation of motion of a simple pendulum:

$$T = mg\cos(\theta)$$

$$m\ddot{x} = mL\ddot{\theta} = -mg\sin(\theta)$$

$$\Rightarrow \ddot{\theta} = -\frac{g}{L}\sin(\theta) = -\frac{g}{L}\theta + \mathcal{O}(\theta^3) \approx -\frac{g}{L}\theta$$

where the last approximation was taken by using the first term in the Taylor expansion, which means is only valid for small angles. This can be conveniently recasted as:

$$\dot{\theta} = \omega$$

$$\dot{\omega} = \ddot{\theta} = -\frac{g}{L}\sin(\theta) = F(\theta, t)$$

So, basically we have a system of two coupled first order ODEs. Now, let's analyze the time dependence of the Energy:

$$\dot{E_{tot}} = \frac{1}{2}mL^2 2\omega\frac{d\omega}{dt} + \frac{1}{2}mgL2\theta(t)\frac{d\theta}{dt} = mL\{L\omega\dot{\omega} + g\theta\omega\}$$

$$= mL\{-L\omega\frac{g}{L}\sin(\theta) + g\theta\omega\} = mL\{-g\sin(\theta)\omega + g\theta\omega\}$$

$$= mLg\omega\{-\sin(\theta) + \theta\} \approx 0$$

where in the last step the small angle approximation was taken. Hence, we just proved that energy is conserved in the pendulum, as long as the starting angle is small.

$$= mLg\omega\{-\sin(\theta) + \theta\} \approx 0$$

Now, to illustrate the difference with the Euler method, we can write this as a set of difference equations:

$$\theta_{n+1} = \theta_n + \Delta t\omega_n + \mathcal{O}(\Delta t^2)$$

$$\omega_{n+1} = \omega_n - \Delta t\frac{g}{L}\sin(\theta) + \mathcal{O}(\Delta t^2)$$

And, we can write the energy of the system after $n+1$ iterations:

$$E^{tot}_{n+1} = \frac{1}{2}mL^2\omega^2_{n+1}(t) + \frac{1}{2}mgL\theta^2_{n+1}(t) - mgL$$

So, by replacing θ_{n+1} and ω_{n+1}:

$$E^{tot}_{n+1} = \frac{1}{2}mL^2(\omega_n + \Delta t\dot{\omega}_n)^2 + \frac{1}{2}mgL(\theta_n + \Delta t\omega_n)^2 - mgL$$

$$E^{tot}_{n+1} = \underbrace{\frac{1}{2}mL^2\omega_n^2 + \frac{1}{2}mgL\theta_n^2 - mgL}_{E_n} + mL^2\omega_n\dot{\omega_n}\Delta t + mgL\theta_n\omega_n\Delta t + \frac{1}{2}mL^2\dot{\omega_n}^2\Delta t^2 + \frac{1}{2}mgL\omega_n^2\Delta t^2$$

$$= E_n + \cancel{mL^2\omega_n(-\frac{g}{L}\theta_n)\Delta t} + \cancel{mgL\theta_n\omega_n\Delta t} + \frac{1}{2}mL^2(-\frac{g}{L}\theta_n)^2\Delta t^2 + \frac{1}{2}mgL\omega_n^2\Delta t^2$$

$$= E_n + \frac{1}{2}mL\left(\cancel{L}\frac{g^2}{\cancel{L^2}}\theta_n^2 + g\omega_n^2\right)\Delta t^2 = E_n + \frac{1}{2}mgL\left(\frac{g}{L}\theta_n^2 + g\omega_n^2\right)\Delta t^2$$

$$\boxed{\Rightarrow E_{n+1}^{tot} = E_n + \frac{1}{2}mgL\left(\frac{g}{L}\theta_n^2 + g\omega_n^2\right)\Delta t^2}$$

Which clearly shows that energy is increasing over each iteration. In figure 1, the increase in the amplitude of the motion is clear. Hence, simulations also show that the Euler method does not conserve energy. The code for the plot was adapted from matlab-pendulum.m given in class.

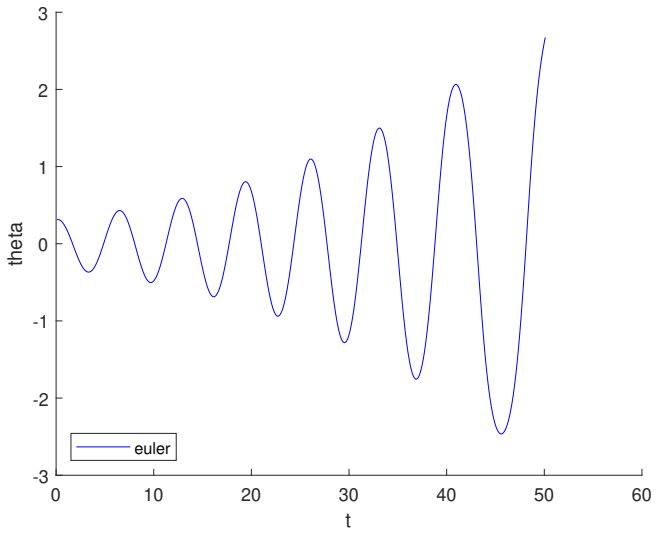

Figure 1: Equation of the motion for the simple pendulum under the small angle approximation using the Euler method. The amplitude is growing over time, meaning that the energy will grow over time. The error can be partially corrected by choosing a small enough step, but it cannot be eliminated.

2 Problem 2

A harmonic oscillator has the equations of motion $\ddot{x} = -\omega^2 x$, with solution $x(t) = x_0 \cos(\omega t) + \frac{v_0}{\omega}\sin(\omega t)$.

(a) **Show that the equation can be non-dimensionalized by using the natural times $\tau = \omega t$. What is the initial velocity in these units?**

$$\ddot{x} = -\omega^2 x \Leftrightarrow \frac{d^2x}{dt^2} = -\omega^2 x$$

In order to make the equation adimensional, we can use the following change of variables:
$\tau = \frac{t}{t_c} \Rightarrow dt = t_c d\tau$
$\chi = \frac{x}{x_c} \Rightarrow dx = x_c d\chi$

$$\Rightarrow \frac{x_c}{t_c^2}\frac{d^2\chi}{d\tau^2} = -\omega^2 x_c \chi$$

$$\Leftrightarrow \frac{\cancel{x_c}}{t_c^2}\frac{d^2\chi}{d\tau^2} = -\omega^2 \cancel{x_c}\chi \Leftrightarrow \frac{d^2\chi}{d\tau^2} = -t_c^2\omega^2\chi$$

$$\Rightarrow t_c^2\omega^2 = 1 \Rightarrow t_c = \frac{1}{\omega}$$

Thus, the change of variables that adimensionalizes the equation is $\tau = \omega t$ and the resulting equation is:

$$\ddot{\chi} = -\chi$$

In this units the initial velocity is:

$$v_0 = \left(\frac{dx}{dt}\right)_{t=0} = \omega x_c \left(\frac{d\chi}{d\tau}\right)_{\tau=0} = \omega x_{max}\left(\frac{d\chi}{d\tau}\right)_{\tau=0}$$

$$\Rightarrow \boxed{\left(\frac{d\chi}{d\tau}\right)_{\tau=0} = \frac{v_0}{\omega x_{max}}}$$

where x_{max} is the amplitude of the oscillator. It is natural to choose this constant to get our system completely non-dimensional since it is one of the characteristics of our system. One might argue that any choice would be good, since x_c is not present in the final reshape of the differential equation (as long as $x_c = 0$), but in my opinion it is better to work with a normalized dimension. For instance, if we consider interatomic forces as oscillators, the displacement would be extremely small ($\approx 10^{-12}$ m). So, not normalizing the distances x might lead to numerical issues.

(b) **Write a program (in your preferred language) that numerically solves the non-dimensionalized harmonic oscillator, $\ddot{x} = -x$, with $x_0 = 0$ and $v_0 = 1$, using both the Verlet and Runge-Kutta 4th order methods. Compute $x^{(verlet)}(T)$ and $x^{(rk4)}(T)$ (the estimated x at time T using the verlet and rk4 methods, respectively), where $T = 5$ and with $\Delta t \epsilon \{0.5, 0.1, 0.05, 0.01, 0.005, 0.001\}$. Plot $g_1(\Delta t) = |\sin(T) - x^{Verlet}(T)|$ and $g_2 = |\sin(T) - x^{rk4N}(T)|$ on log-log axes and comment on any differences between them.**

Figure 2 shows the approximation for different time steps and the absolute error as a function of the time step. The advantage of 4th order Rung-Kutta(rk4) over Verlet(verlet) is evident as its associated error decreases faster with smaller time steps. From the $g1/g2$ plot, it is clear that the error is about one order of magnitude smaller for rk4 than for verlet. However, below the values suggested in the problem, we start seeing numerical approximation errors due to the finite precision on the computing machine, as shown in figure 2 bottom right.

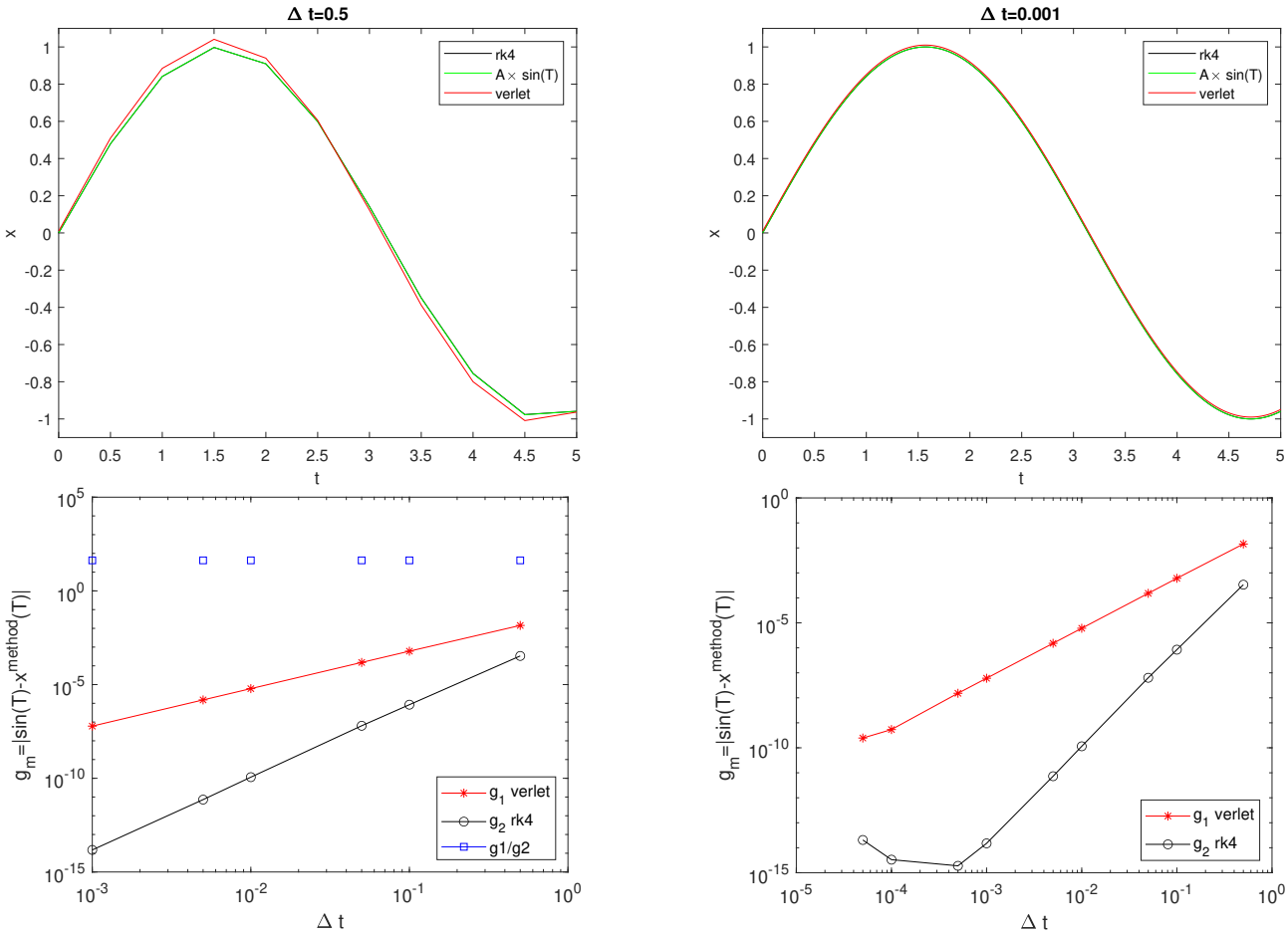

Figure 2: Top left: Approximation with a time step of 0.5. Top right: Approximation with time step 0.001. Bottom left: approximation error as a function of time step size. Bottom right:approximation error as a function of time step size for smaller time steps showing numerical problems. Clearly, rk4 becomes more and more precise for smaller time steps until we reach numerical problems below 10^{-3}.

3 Problem 3

The Korteweg-de Vries (KdV) equation describes wave motion in shallow water, with the normalized height $u(x,t)$ satisfying the PDE:

$$\frac{\partial u}{\partial t} + 6u(x,t)\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0$$

(a) **Show that the KdV equation permits the solutions $u(x,t) = v(x-ct)$, and reduces to the ordinary differential equation $-cv'(y) + 6v(y)v'(y) + v'''(y) = 0$ with this substitution.**

If we let $u(x,t) = v(x-ct) = v(y)$ where $y = x - ct$, the derivatives of u are:

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial y}\frac{\partial y}{\partial t} = -c\frac{\partial v}{\partial y}$$

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial v}{\partial y}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)\frac{\partial y}{\partial x} = \frac{\partial^2 v}{\partial y^2}$$

$$\frac{\partial^3 u}{\partial x^3} = \frac{\partial}{\partial y}\left(\frac{\partial^2 u}{\partial x^2}\right)\frac{\partial y}{\partial x} = \frac{\partial^3 v}{\partial y^3}$$

$$\Rightarrow -c\frac{\partial v}{\partial y} + 6v\frac{\partial v}{\partial y} + \frac{\partial^3 y}{\partial y^3} = 0 \Leftrightarrow \boxed{-cv'(y) + 6v(y)v'(y) + v'''(y) = 0}$$

(b) **Show that the steady-state KdV equation can be made parameter-free (no c) by substituting $y = z/\sqrt{c}$ and $v(y) = cw(z)$**

Let's define adimensional parameters $w = v/v_c$ and $z = y/y_c$. Then, the differential equation becomes:

$$-c\frac{\cancel{v_c}}{\cancel{y_c}}\frac{\partial w}{\partial z} + 6\cancel{v_c}w\frac{v_c}{\cancel{y_c}}\frac{\partial w}{\partial z} + \frac{\cancel{v_c}}{y_c^{\cancel{3}2}}\frac{\partial^3 y}{\partial z^3} = 0$$

$$-\frac{\partial w}{\partial z} + 6\frac{v_c w}{c}\frac{\partial w}{\partial z} + \frac{1}{cy_c^2}\frac{\partial^3 y}{\partial z^3} = 0$$

So, the choice becomes clear:

$$\frac{v_c}{c} = 1 \Rightarrow v_c = c$$

and,

$$\frac{1}{cy_c^2} = 1 \Rightarrow y_c = \sqrt{\frac{1}{c}}$$

Hence, the change of variables adequate to non-dimensionalize our system are are: $w = v/c$ and $z = \sqrt{c}y$.

(c) **Use rk4 to solve the parameter-free KdV equation, $w''' = (1-6w)w'$, with $w(0) = 1/2$, $w'(0) = 0$, and $w''(0) = -1/4$, for $z\epsilon(0,5)$. Plot your numerical result as points in the same figure as the exact solution to this nonlinear equation, $w_{exact} = \frac{1}{2}sech^2(z/2)$.**

By modifying the course code, the solution for the equation was implemented. The code is in the GitHub and figure 3 shows the results for the given parameters.

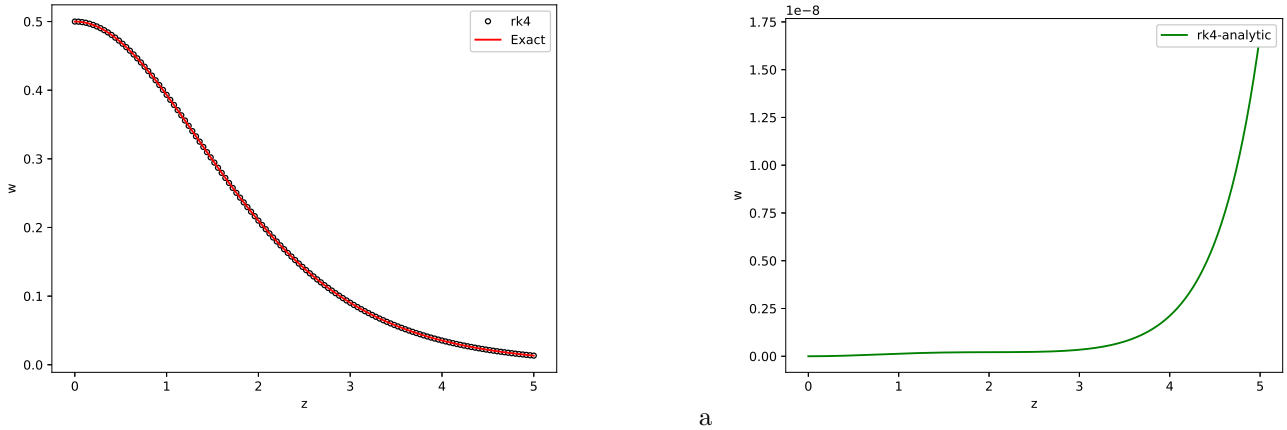

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Figure 3: Left: Approximation using rk4 showing the very good match between the theoretical answer and the numerical implementation. Right: Difference between the approximation and the analytical answer, it shows how the difference start increasing for larger times.

(d) **Repeat your numerical integration over the domain $z\epsilon(0, 50)$, and plot your computed $w(z)$. You should observe a sequence of "solitons": localized traveling peaks in the fluid that are well separated. The KdV was the first model to successfully describe experimentally observed solitons in water.**

This part illustrates what we mentioned on (c), that the error starts increasing after certain point. By lowering the step size we can "delay" the appearance of this bumps and maintain a good approximation to the solution. However, the computational cost or numerical problems will become an issue at certain point. It is worth noting that the numerical solution carries very special features, it is a periodic solution where "solitons" appear. That is, this equation, for certain parameters can be used to describe periodic pulses. However, this are not features of the analytical approximation but appear only on the discretized solution.

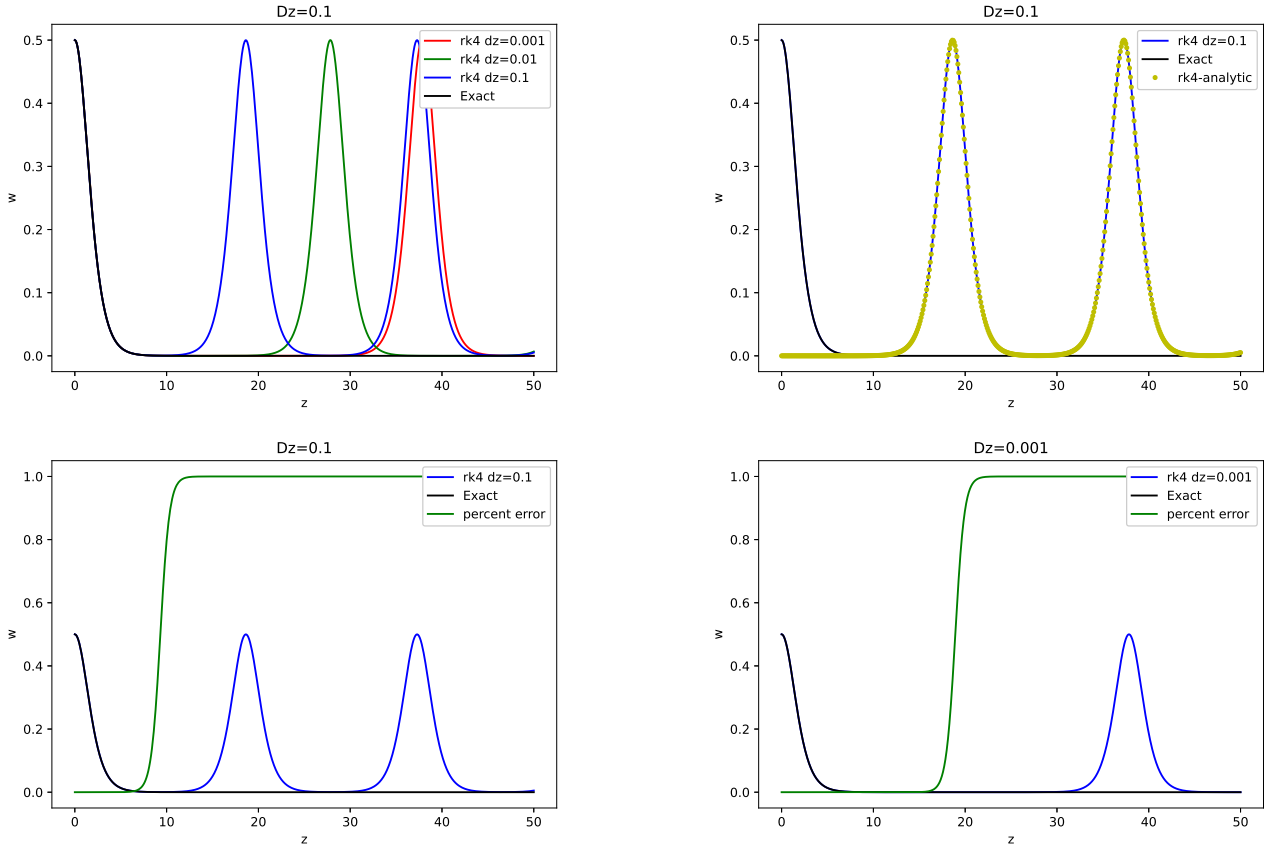

Figure 4: Top left: Approximation using rk4 showing the presence of bumps in the numerical solution. The position and number of bumps depend on the step size. Top right: Difference between the approximation and the analytical answer, it shows that the analytical solution basically becomes zero after $t \approx 10$. Bottom left: The percent error becomes nearly one around $t \approx 12$. Bottom right: For a smaller step size the appearance of the error is "delayed". However, further lowering the step size carries high computational costs and numerical issues.