PHYS 381 – Midterm Assignment

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Scientist #1: Finding the minima of a potential.

a) We know that the bottom of a potential well is a point of stable equilibrium. Therefore, we need to find the set of conditions that shows us the bottom of a plot of the function $V(r) = 4 \in \{(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}\}$. The best way to show this is mathematically. We first need to derive V(r) with respect to r:

$$V(r) = 4 \in \left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\} = 4 \in r^6\{\frac{r^6 - r^6}{r^{12}}\}$$

Taking the derivative:

$$\frac{dV(r)}{dr} = 4 \in r^6\{\frac{-6r^5(r^{12}) - 12r^{11}(r^6 - r^6)}{r^{24}}\}$$

$$= 4 \in r^6\{\frac{6(-2r^6 + r^6)}{r^{13}}\}$$

The most stable condition is when the Derivative is set to zero.

$$\frac{dV(r)}{dr} = 0 = \frac{24 \in r^6(-2r^6 + r^6)}{r^{13}}$$

Multiplying all constants across and reorganizing we end up with the stable state for this potential:

$$\frac{dV(r)}{dr} = 0 = -2r^6 + r^6$$

The stable state for this potential is when the derivative is set to zero, as shown above. From here any calculations needed for the stable potential can be performed.

b) This problem can best be solved with the aid of a computer. Although not an exact solution, it is necessary to use a computer as an analytical solution is not available for this problem. A computer algorithm of this problem is more efficient for determining the minima of this potential. Instead of solving the exact potential given, we will solve a similar problem in which the root is to be found one time, $|F(x)| < N$ where N is a small number chosen. To obtain the exact result using a computer based numerical method we would have to guess the exact root as the initial condition. The more steps taken in the iterations through numerical methods, the more accurate the approximation will be.

c) While both the Bisection method and the Newton Raphson method could be used to solve this problem, they are different, and each have their own strengths. For this problem it would be best to use the Newton Raphson method. The Newton Raphson method is ideal for this problem as we already have the information required. The newton Raphson method follows the expansion of a Taylor's series about a specific point $x = x_0 + \in$. Setting $f(x_0 + \in) = 0$, we get $x_0 + \in$ as an approximation for a root. Now that we have this condition in place, we can now see that $F(x_0) + F'(x_0) \in= 0$, where $\in= -\frac{F(x_{0)}}{F\prime(x_{0)}}$, being the first order adjustment to the root. Finally, we can set $x_1 = x_0 + \in$, with this process iterating until it converges to a point close to the actual root using the final function $x_{n+1} = x_n - \frac{F(x_{n)}}{F\prime(x_n)}$ where n is the number of iterations. The Newton Raphson method is more efficient and accurate than the bisection method and the above steps give a good starting point. Using both methods for other problems, it should be noted that the Bisection Method is easier to use and requires less initial information whereas the Newton Raphson method is more challenging to use and requires more initial information. The Newton Raphson method is the best choice for this problem.

d) The plots described look good. The potential function is correct, and the derivative of this function is also correct. There are a few ways that these plots could be improved. It is rather difficult to see the actual result as a point as there are multiple points plotted together close by. The ambiguous non root points should be removed and only the minima at 3.816370 should be plotted for each graph. Also, considering we are specifically looking at the minima as the result, not the whole graph, it might be beneficial to zoom in more on the actual minima rather than showing the ends of the function. Perhaps setting the x values to 2 < x < 6 and the y values to -2 < y < 2 would better represent the minima.

Scientist #2: Nonlinear System of Equations.

a) It is important to note that the Lorenz System provided in this problem cannot be solved analytically using integration. Instead, this problem can be tackled using the Runge-Kutta Method or the Trapezoid method. Specifically, for this problem, the Runge-Kutta method should be implemented. The Runge-Kutta method is like the Trapezoid method except the Taylor Series expansion is carried out at the middle point of the time steps. The Runge-Kutta method proves to be better than the Trapezoid method for this problem as the approximation is done at ΔT^2 rather than at ΔT. This allows the Runge-Kutta method to be greatly more accurate when solving a system of linear equations, specifically the Lorenz System given in this problem. This is because the Runge-Kutta method, especially at higher orders, is reliable with higher T and dT values compared to the Trapezoid method, which often falls off with these higher T and dT values. A simple starting point for the Runge-Kutta method is to choose an initial state, an arbitrary point in three-dimensional space, and then calculating a few derivatives proportionally based on the order of the Runge-Kutta chosen. We then combine the derivatives and using a chosen time step *n*, to calculate an approximation for the next point and repeat.

b) For this problem it will first be beneficial to show the difference between the second and fourth degree Runge-Kutta methods and then analyze the best solution for the Lorenz System provided. The Runge-Kutta method estimates multiple numbers of slopes based on the order seeking. In simple terms for a second order Runge-Kutta method, we must start with a first order differential equation:

$$\frac{dy(t)}{dt} = f(y(t), t)$$

We then progress through a point at Y'(t) one step at a time, let us define the steps as n:

$$k_1 = f(y'(t_0), t_0)$$

$$y_1(t_0 + n) = y'(t_0) + k_1 n$$

We then do the same thing for each order; in our case we are trying to find the second order, so we do it once more to finally obtain:

$$y'(t_0 + n) = y'(t_0) + n\frac{(k_1 + k_2)}{2}$$

This is the second order Runge-Kutta method, which uses the same equivalent distance of start and end point. Let us now examine the fourth order Runge-Kutta method we will start with the same first order differential equation:

$$\frac{dy(t)}{dt} = f(y(t), t)$$

As above, we progress through a point at Y'(t) one step at a time, with steps being n:

$$k_1 = f(y'(t_0), t_0)$$

$$y_1(t_0 + n) = y'(t_0) + k_1 n$$

We want to do the same thing until we reach the desired order, in this case the fourth order which will obtain this result:

$$y'(t_0 + n) = y'(t_0) + n\frac{(k_1 + 2k_2 + 3k_3 + k_4)}{6}$$

The fourth order Runge-Kutta method is more accurate as it breaks the problem into more small steps. We introduce a greater difference between the steps which allows for more calculations to occur with more specific time steps. It also allows for more slopes to be calculated and when combined we are left with a better estimation. Although it may take more time if it were to be done by hand, since we are doing it with a computer it will not be a problem.

c) It is important to note that small changes in initial conditions can cause catastrophic result differences. Even something as small as to the negative tenth power. There actually is a phenomenon in the physics world for this – chaos theory, specifically the butterfly effect.

When considering chaos theory and the butterfly effect, it is important to note that chaotic motion problems are highly responsive to small changes in initial conditions. The Lorenz system is known to create chaotic conditions, so therefore we are seeing these abnormalities in the results when the random fluctuations are added. Assuming the Runge-Kutta method was chosen to solve this problem, since it breaks the problem apart into extremely small slopes and estimations for better accuracy. Each estimation is so close to the others especially for the initial conditions even though we know that the results will not be this close together. This is another reason why changes in initial conditions can cause drastic changes in the results.

References:

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