PHYS 7810: Practicum 1

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Derivation of the core equation

The Crank-Nicolson method works by equally sampling the forward euler method at a given point n and the backward euler scheme at $n+1$. In essence, we end up using the value of $f\left(x_{mid}\right)$ where x_{mid} is at the 'midpoint' between x_n and x_{n+1}. For the simple harmonic oscillator, we have the following two differential equations:

$$\dot{v} = -\omega_0^2 x$$

$$\dot{x} = v$$

Sampling v at the midpoint between n and $n+1$ yeilds the following:

$$x_{n+1} - x_n = \frac{h}{2}\left(v_{n+1} + v_n\right)$$

Where h is the step size. Similarly, for v, we have

$$v_{n+1} = v_n + hf\left(\frac{x_{n+1} + x_n}{2}\right) = v_n + hf\left(x_n + \frac{h}{4}\left[v_{n+1} + v_n\right]\right)$$

where $f\left(x\right) = -\omega_0^2 x$. It makes sense to solve for v_{n+1}first, since it only depends on x_n and v_n. In essence,

$$v_{n+1} = v_n - h\omega_0^2\left(x_n + \frac{h}{4}\left[v_{n+1} + v_n\right]\right)$$

$$\implies v_{n+1}\left[1 + \frac{\omega_0^2 h^2}{4}\right] = v_n\left[1 - \frac{\omega_0^2 h^2}{4}\right] - h\omega_0^2 x_n$$

Thus,

$$v_{n+1} = \frac{v_n\left[1 - \frac{\omega_0^2 h^2}{4}\right] - h\omega_0^2 x_n}{1 + \frac{\omega_0^2 h^2}{4}}$$

Once v_{n+1} is known, we can simply plug it into the x equation to get

$$x_{n+1} = x_n + \frac{h}{2}\left(v_{n+1} + v_n\right)$$

thus giving us x and v for each time step

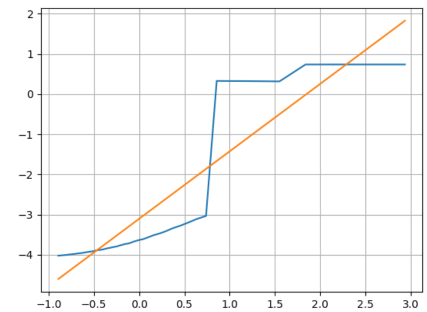

Figure 1: Zero crossing measurement done for between 2 and 45 points between 0 and 6π. The x axis of the log-log plot is the step size while the y axis is the error in the frequency $|f_{measured} - \omega_0/2\pi|$

Additional optimizations made

- Since floating point multiplication is much faster than floating point division, the divisor in the v equation, $1/\left(1 + \frac{\omega_0^2 h^2}{4}\right)$ was computed seperately outside the loop and at each timestep, this variable 'pdt2om2' in crank_nicolson.py was multiplied with the numerator.

Zero Crossing Loop

To measure the zero crossing of the solution, $x[i]$ was looped over i till the sign of x changed. If this condition turned out to be true, the time of the zero crossing was taken to be the midpoint of the line connecting $x[i]$ and $x[i-1]$ as follows:

$$t_{cross} = t[i-1] + \frac{t[i] - t[i-1]}{|x[i] - x[i-1]|}(x[i-1])$$

The absolute value is simply so that we can treat $x[i] > x[i-1]$ and $x[i-1] > x[i]$ the same, thus removing one extra if condition. We do not need to do this for $t[i] - t[i-1]$ since t always increases.

Results of the Zero-Crossing measurement

For the chart obtained in figure 1, the least squares fit was the following: $x = 1.6802t - 3.1057$. However, as the number of data points increased, the error in frequency stabilized at $\ln|f_{error}| \sim -4.1$, suggesting that we're now hitting the limit of either the interpolation in the zero-crossing measurement or the true limit of the method, $O\left((dt)^2\right)$. To verify this, the least squares line for the frequency plot was obtained exclusively with coarser grids and the tapering limit appeared to be $m_{lsq} \sim 2$, suggesting that this was indeed the frequency error of the method $O\left((dt)^2\right)$. A better way to verify this would be to interpolate with three points to find the zero crossing and see if this limit is preserved.