PHY 407 Lab 7

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1 Question 1

For the implicit trapezoid method, we can derive the growth factor for ODE $dy/dt = \lambda y = f(y)$ starting from the expression for the $k+1$th point in terms of the kth point.

$$\begin{aligned}
y_{k+1} &= y_k + \frac{h_k}{2}[f(y_k) + f(y_{k+1})] \\
y_{k+1} &= y_k + \frac{h_k}{2}[\lambda y_k + \lambda y_{k+1}] \\
\left(1 - \lambda\frac{h_k}{2}\right) y_{k+1} &= \left(1 + \lambda\frac{h_k}{2}\right) \\
y_{k+1} &= \left[\frac{1+\lambda\frac{h_k}{2}}{1-\lambda\frac{h_k}{2}}\right] y_k \\
y_{k+1} &= \left[\frac{1+\lambda\frac{h_k}{2}}{1-\lambda\frac{h_k}{2}}\right]^k y_0
\end{aligned}$$

Our stability constraint requires the absolute value of the growth factor to be less than one. In this case the growth factor is:

$$\frac{1+\lambda\frac{h_k}{2}}{1-\lambda\frac{h_k}{2}}.$$

This means our condition on stability is:

$$\left|\frac{1+\lambda\frac{h_k}{2}}{1-\lambda\frac{h_k}{2}}\right| \leq 1 \tag{1}$$

$$\left|1+\lambda\frac{h_k}{2}\right| \leq \left|1-\lambda\frac{h_k}{2}\right|$$

In terms of the two parameters λ and h_k, we have shown that the solution is stable iff $\lambda h_k \leq 0$. However, since a zero step size is meaningless from a computational perspective and $\lambda = 0$ gives our ODE a trivial solution, we can logically restrict to stable solutions with $\lambda h_k < 0$. This means that we have the following set of conditions:

$$\begin{aligned}
&\text{if} \quad \lambda < 0, \text{ then } h_k > 0 \\
&\text{if} \quad h_k < 0, \text{ then } \lambda > 0
\end{aligned}$$

The Taylor expansion of $y(t+h)$ is given by:

$$\begin{aligned}
y(t+h) &= y(t) + hy'(t) + O(h^2) \\
&= y(t) + hf(y(t), t) + O(h^2) \\
\implies y(t_{k+1}) &= y(t_k) + h_k \lambda y(t_k) + O(h_k^2)
\end{aligned}$$

Subtract this from the expression for y_{k+1}:

$$y_{k+1} - y(t_{k+1}) = \left[\frac{1 + \lambda \frac{h_k}{2}}{1 - \lambda \frac{h_k}{2}} \right] y_k - (1 + h_k \lambda) y(t_k) + O(h_k^2)$$

If we attempt to find the local error l by assuming no error prior to the $k+1$ step, we find:

$$\begin{aligned}
y_{k+1} - y(t_{k+1}) &= \left[\frac{1 + \lambda \frac{h_k}{2}}{1 - \lambda \frac{h_k}{2}} \right] y_k - (1 + h_k \lambda) y_k + O(h_k^2) \\
y_{k+1} - y(t_{k+1}) &= \left[\frac{1 + \lambda \frac{h_k}{2}}{1 - \lambda \frac{h_k}{2}} - (1 + \lambda h_k) \right] y_k + O(h_k^2) \\
y_{k+1} - y(t_{k+1}) &= \left[\frac{1 + \lambda \frac{h_k}{2} - (1 + \lambda h_k)(1 - \lambda \frac{h_k}{2})}{1 - \lambda \frac{h_k}{2}} \right] y_k + O(h_k^2) \\
y_{k+1} - y(t_{k+1}) &= \left[\frac{1 + \lambda \frac{h_k}{2} - 1 + \lambda^2 \frac{h_k^2}{2} - \lambda h_k + \lambda \frac{h_k}{2}}{1 - \lambda \frac{h_k}{2}} \right] y_k + O(h_k^2) \\
y_{k+1} - y(t_{k+1}) &= \left[\frac{\lambda^2 \frac{h_k^2}{2}}{1 - \lambda \frac{h_k}{2}} \right] y_k + O(h_k^2) \qquad (2)
\end{aligned}$$

Given that if $l = O(h_k^{p+1})$ then that accuracy is p, it should be possible to determine from Equation 2 the accuract of the implicit trapezoid method, however I am not sure how to interpret my result.

2 Question 2

Comparing Figure 1 and Figure 2 makes it obvious that integration with a fixed step size requires many more points of evaluation. As expected, in Figure 1, spacing between evaluation points becomes smaller in regions where the function changes quickly, and spreads out where the functions change slowly.

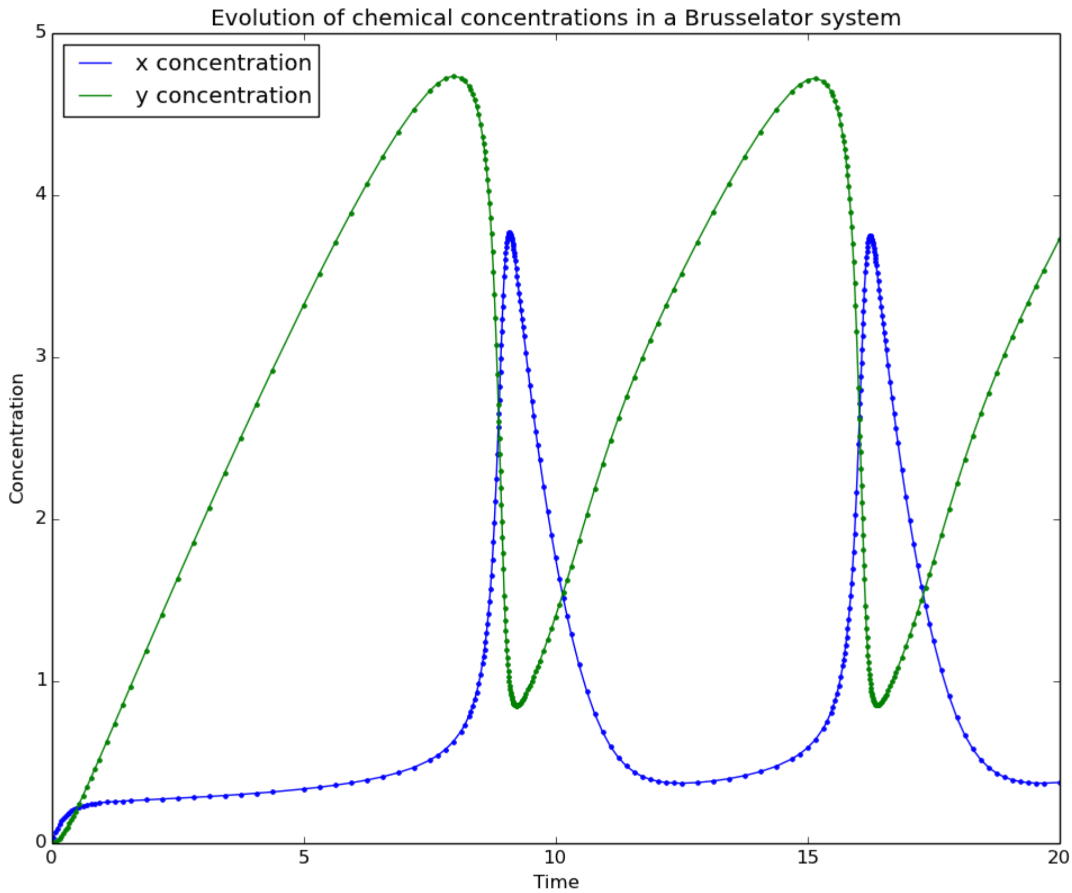

Figure 1: Concentrations over time computed using an adaptive step size

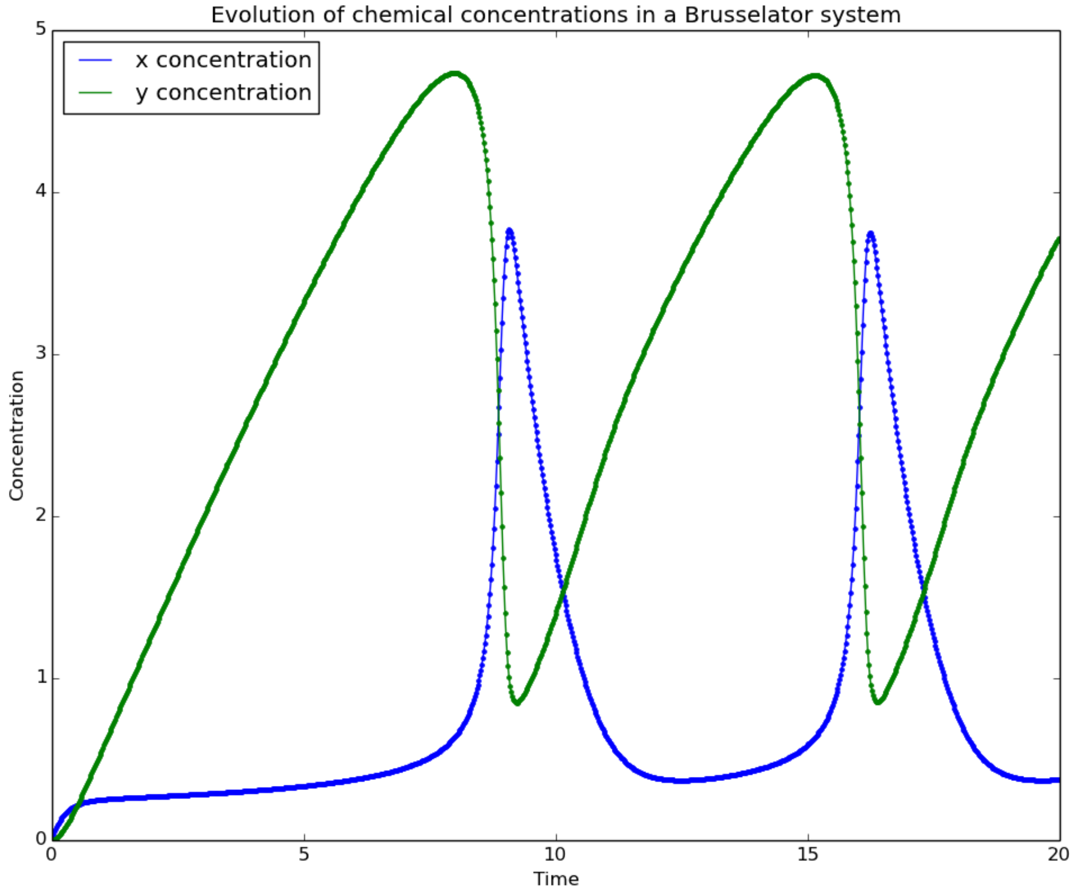

Figure 2: Concentrations over time computed using an fixed step size

3 Question 3

Denote the ground state with the index 0, and the nth excited with the index n. Then the energy eigenvalues of the harmonic potential Hamiltonian in a square box are as follows.

$$\begin{aligned} E_0 &= 138.024\,\text{eV} \\ E_1 &= 414.072\,\text{eV} \\ E_2 &= 690.120\,\text{eV} \end{aligned}$$

The difference between pairs of sequential values is 276.048 eV, so the the energy eigenvalues are equally spaced, as expected.

4 Question 4

Denote the ground state with the index 0, and the nth excited with the index n. Then the energy eigenvalues of the anharmonic potential Hamiltonian in a square box are as follows.

$$
\begin{aligned}
E_0 &= 205.307\,\text{eV} \\
E_1 &= 735.691\,\text{eV} \\
E_2 &= 1443.569\,\text{eV}
\end{aligned}
$$

5 Question 5

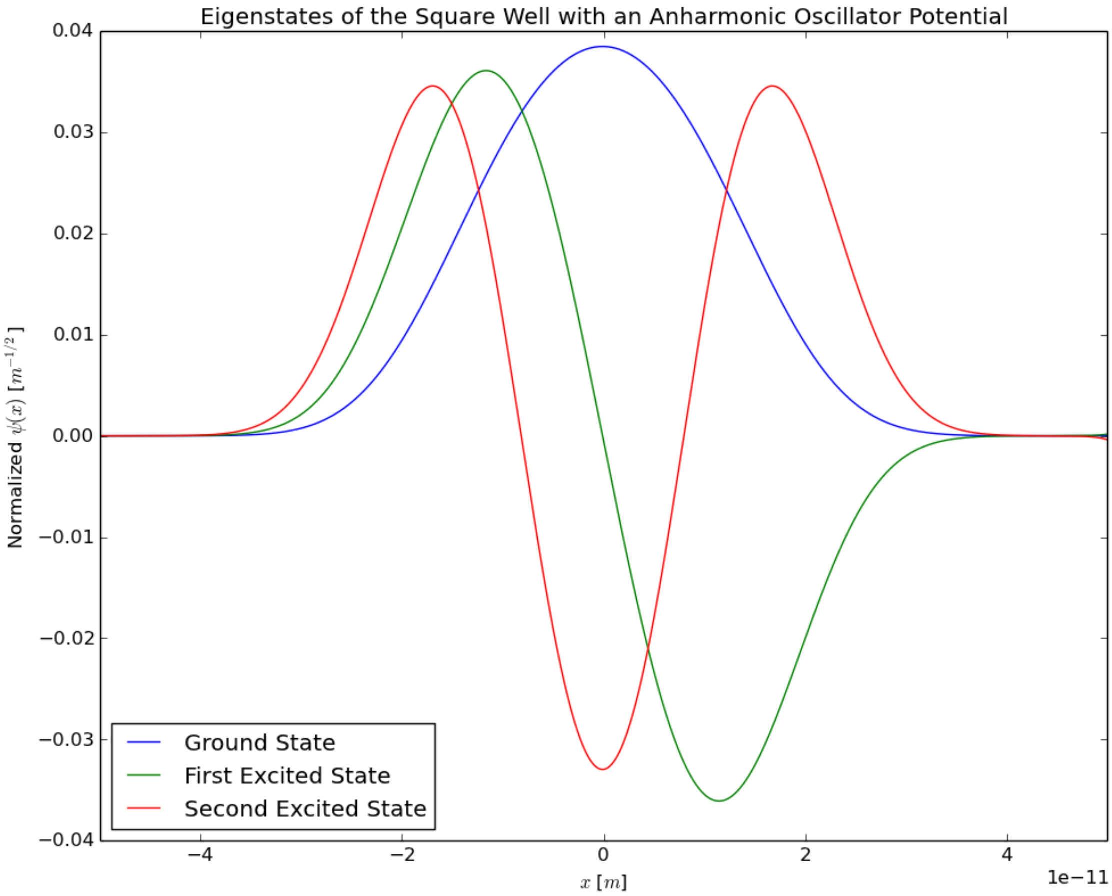

Figure 3