Modeling the Oscillation of Belousov-Zhabotinsky Reaction

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Introduction/Motivation

- Ilya Prigogine formulated a mathematical model of chemical oscillators, known as ‘Brusselator’
- Belousov–Zhabotinsky (BZ) reactions are examples of these oscillators
- When heated, chemicals in BZ reactions undergo a series of changes that cause the chemical concentrations in the mixture to oscillate between two extremes
- These reactions are important because they show that chemical reactions do not have to be dominated by equilibrium thermodynamic behavior, as they are far from equilibrium and remain so for significant periods of time

Equations of Model

$$\frac{dx}{dt} = 1 - (b+1)x + ax^2y$$

$$\frac{dy}{dt} = bx - ax^2y$$

- Equations consist of two constants, a and b, and two variables, x and y, which represent the concentrations of two chemicals involved in the reaction
- x and y initially at 0 and a = 1, b = 3
  - Also varied a to 2 and 3 to see the difference in plots

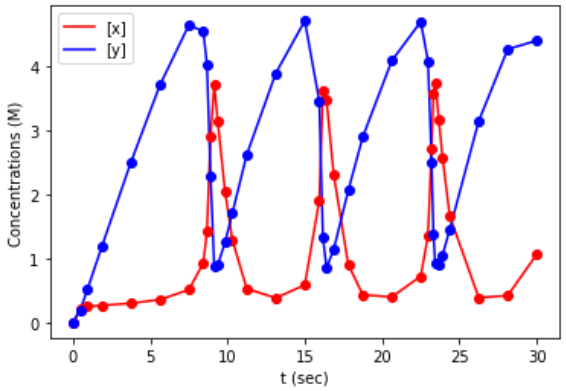
Computational Results

- The concentrations change through time, and the value of the constants act as dampening effects on the oscillation
- With a=1, the oscillation appears undamped

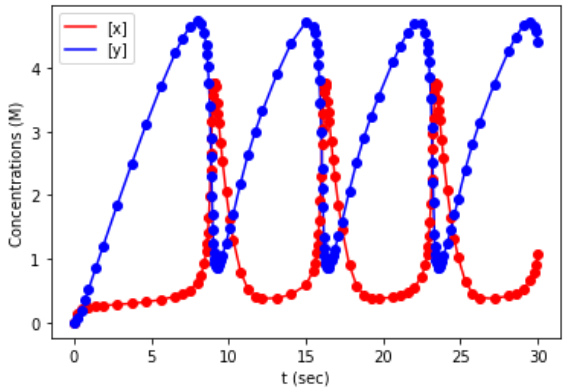
Numerical Modeling Method

- Used the Bulirsch–Stoer method
  - utilizes Richardson extrapolation and the modified midpoint method
- Involves increasing the number of steps until the error on our best estimate at the final step is as small as we want it to be
  - When our error falls below this value the calculation is finished
  - And the solution plot smoothens as the value of delta tends towards zero
- Main limitation is that only the final value is a really accurate answer, all the intermediate points being midpoint method estimates

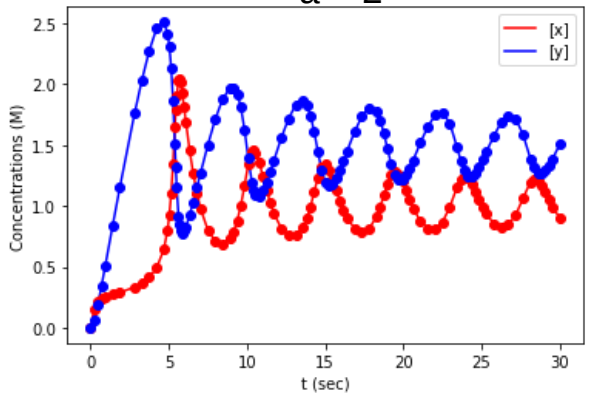
Loose error restriction



a = 1



a = 2



a = 3