Project #1:
The Belousov-Zhabotinskii reaction

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General problem

- **Oscillating chemical system:**
  - the composition may oscillate depending on the initial concentrations

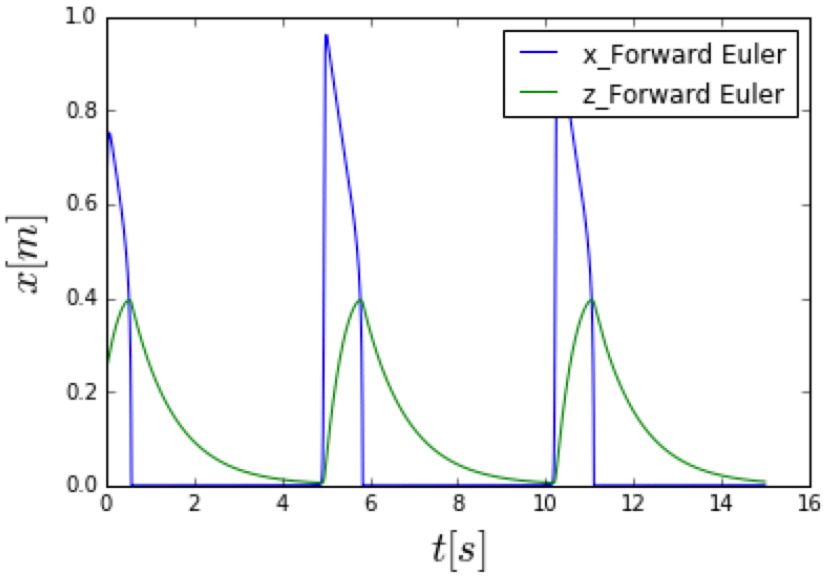
- **Belousov-Zhabotinskii reaction**
  - Oscillating equilibrium between two species:
    - reduction of Cerium(IV) in Cerium(III) by hypobromic acid
    - Oxidation of Cerium(III) into Cerium (IV) by bromate

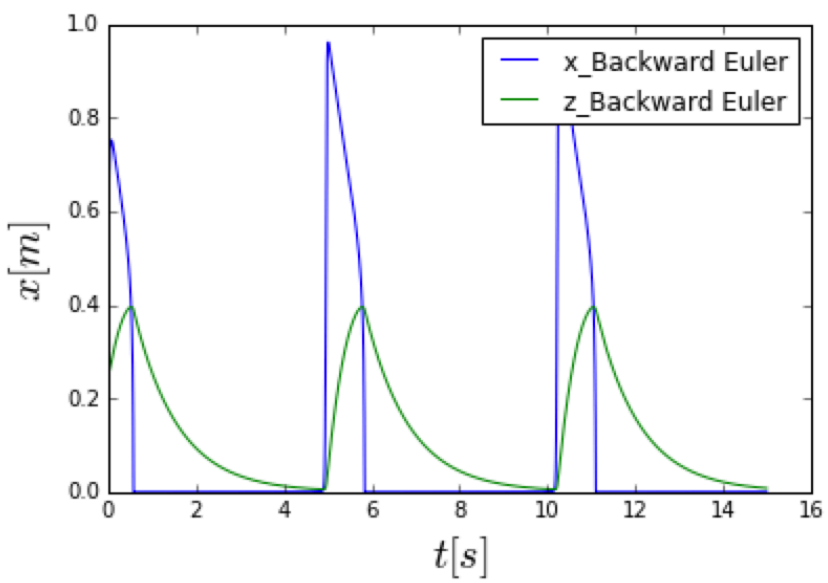
- **Simplified system x=Cerium(IV), y=hypobromic acid**
  - two parameters: f and ϵ

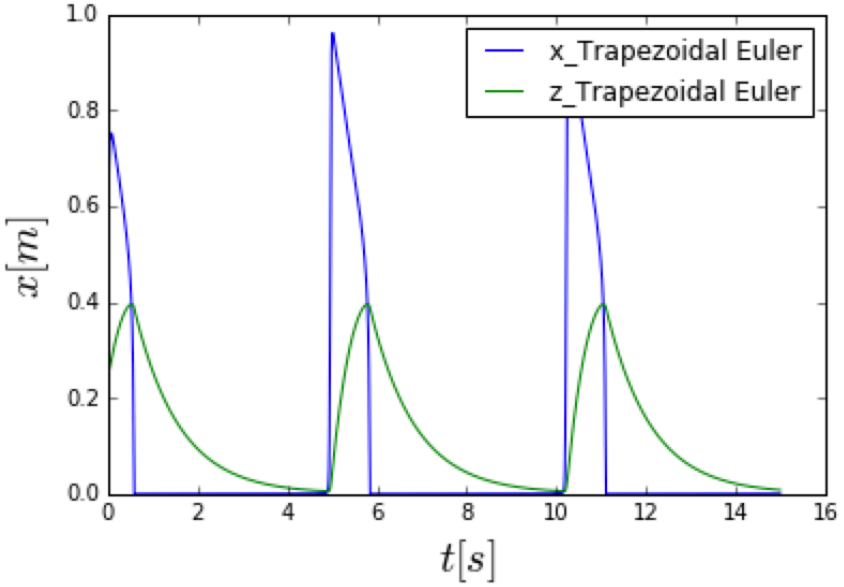
Analysis

- Equation of concentration $\begin{cases} \epsilon \frac{dx}{dt} = x(1-x) + f\frac{q-x}{q+x} z \\ \frac{dz}{dt} = x - z \end{cases}$
- Three methods to apply:
  - Euler forward $\begin{cases} \epsilon \frac{x_{i+1}-x_i}{dt} = x_i(1-x_i) + \mathrm{f}\frac{q-x_i}{q+x_i} z_i \\ \frac{z_{i+1}-z_i}{dt} = x_i - z_i \end{cases}$
  - Euler backward $\begin{cases} \epsilon \frac{x_{i+1}-x_i}{dt} = x_{i+1}(1-x_{i+1}) + \mathrm{f}\frac{q-x_{i+1}}{q+x_{i+1}} z_{i+1} \\ \frac{z_{i+1}-z_i}{dt} = x_{i+1} - z_{i+1} \end{cases}$ → The equation is non-linear, we can not solve directly, we use "fsolve" insteadly.
  - Trapezoidal $\begin{cases} \epsilon \frac{x_{i+1}-x_i}{dt} = ((x_i(1-x_i) + \mathrm{f}\frac{q-x_i}{q+x_i} z_i) + (x_{i+1}(1-x_{i+1}) + \mathrm{f}\frac{q-x_{i+1}}{q+x_{i+1}} z_{i+1}))/2 \\ \frac{z_{i+1}-z_i}{dt} = ((x_i - z_i) + (x_{i+1} - z_{i+1}))/2 \end{cases}$

Result







- The change of x and z are oscillating.
- For z, z(max)=0.396, z(min)=0.06