Chemistry 4010 Lecture 6: Period-doubling bifurcations and chaos

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Example: The Willamowski-Rössler model

$$\mathrm{A}_1 + \mathrm{X} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2\,\mathrm{X}$$

$$\mathrm{X} + \mathrm{Y} \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} 2\,\mathrm{Y}$$

$$\mathrm{A}_5 + \mathrm{Y} \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} \mathrm{A}_2$$

$$\mathrm{X} + \mathrm{Z} \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} \mathrm{A}_3$$

$$\mathrm{A}_4 + \mathrm{Z} \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} 2\,\mathrm{Z}$$

The A_i species are "pool" species, assumed fixed.

Willamowski and Rössler, *Z. Naturforsch. A* **35**, 317 (1980)

Example: The Willamowski-Rössler model

Dimensionless model equations

$$\dot{x} = x(a_1 - k_{-1}x - z - y) + k_{-2}y^2 + a_3$$
$$\dot{y} = y(x - k_{-2}y - a_5) + a_2$$
$$\dot{z} = z(a_4 - x - k_{-5}z) + a_3$$

Let's study these equations with XPPAUT!

Willamowski and Rössler, *Z. Naturforsch. A* **35**, 317 (1980)

Things we learned from this example

Period-doubling bifurcation: bifurcation of a limit cycle in which the period doubles

Period-doubling cascade: often, period-doubling bifurcations are repeated over a finite parameter interval

Sensitive dependence on initial conditions: Exponential divergence of trajectories over time

Chaotic solution characterized as follows:

- Non-periodic solution in a bounded region of phase space
- Displays sensitive dependence on initial conditions
- Fractal attractor
- Often reached as the accumulation of a period-doubling cascade