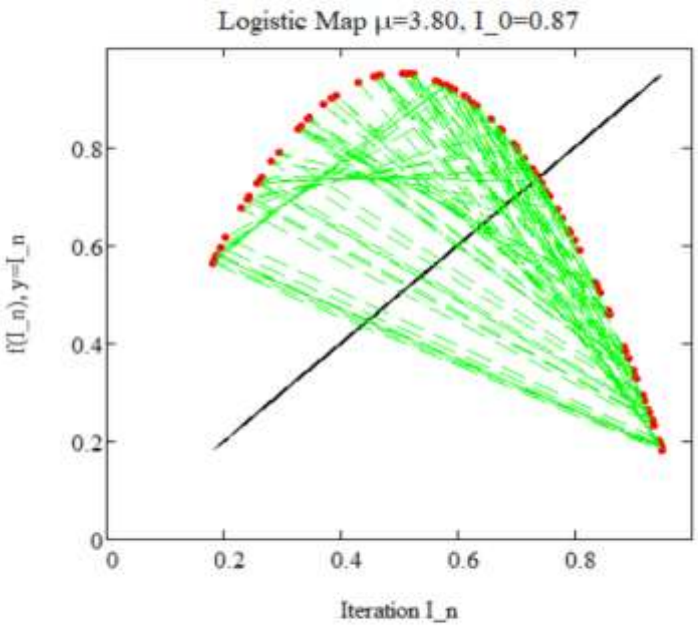
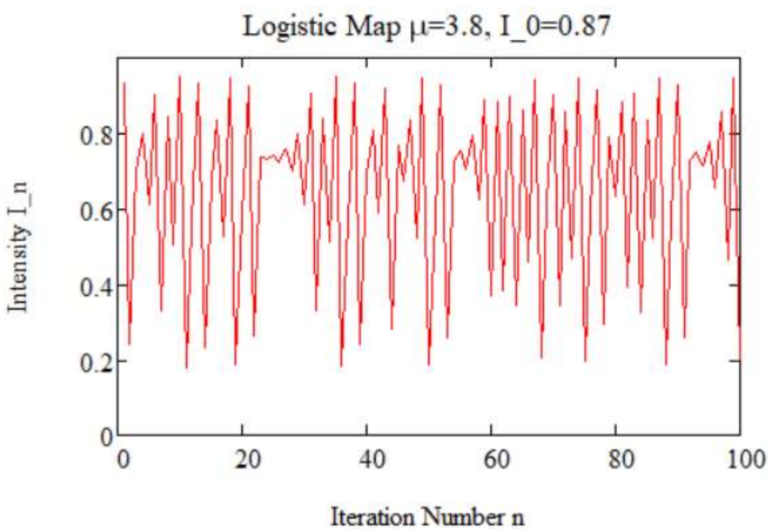
Chaotic Map Trajectories



Same example as before, plot showing only the iterative intensities I_n on the curve representing the map profile function $f(I)$.

A large part of the brightness spectrum is covered by the trajectory already after 500 iteration.
No apparent repetitive intensity pattern.

Intensity flashes between bright and dim.



Same example as above, plot shows iterative intensities I_n vs n. Some, but not exact similarities, intermittency domains, strongly dependent on initial condition I_0.

Sensitivity to Initial Conditions

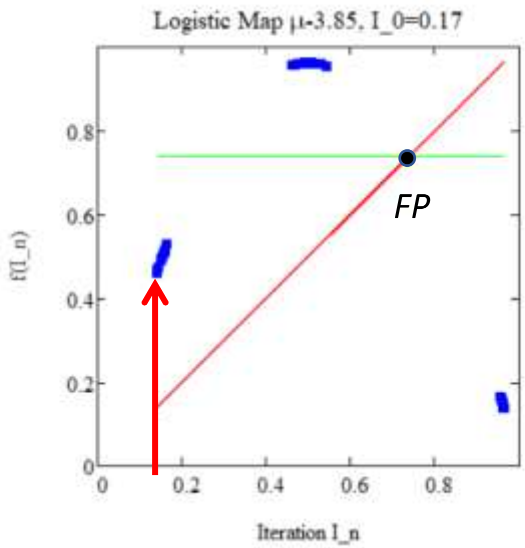


Illustration of sensitivity to initial conditions for

μ = 3.85, fixpoint at *I = 0.74, strange attractor*

IC: I_0 = 0.17, *N* = 100 iterations

Blinking alternatively with 3 different intensities

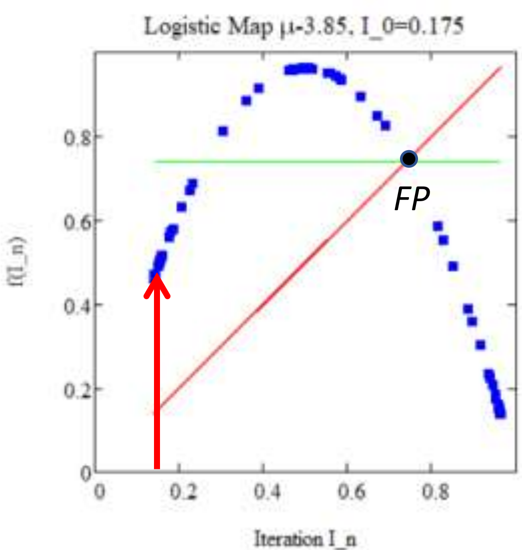


Illustration of sensitivity to initial conditions for

μ = 3.85, fixpoint at *I = 0.74, strange attractor*

IC: I_0 = 0.175, *N* = 100 iterations

Blinking alternatively with a continuum of intensities filling most of the accessible intensity range

Agenda: Complex Processes in Nature and Laboratory

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Reading Assignments Weeks 1&2

LN II: Complex processes

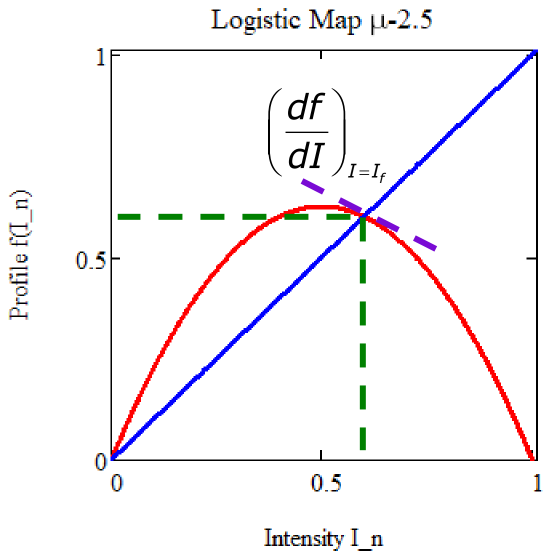
Kondepudi Ch.19

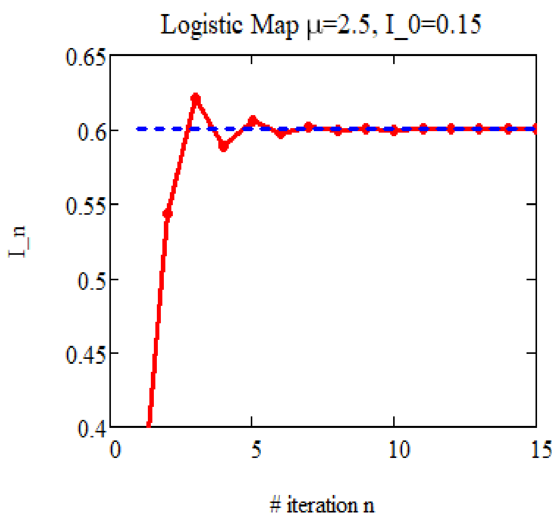
Additional Material

J.L. Schiff: Cellular Automata, Ch.1, Ch. 3.1-3.6

McQuarrie & Simon Math Chapters MC B, C, D,

Logistic Map Features





Profile function *f*, amplification factor $\boldsymbol{\mu}$

$\textit{Fixpoints } I_f : f(I_f) = I_f \qquad \textit{Trivial } I_f = 0$

$\textit{Non-trivial FP exists for } \mu > 1$

$\textit{Trajectory ensembles with } I_0 \approx I_f$

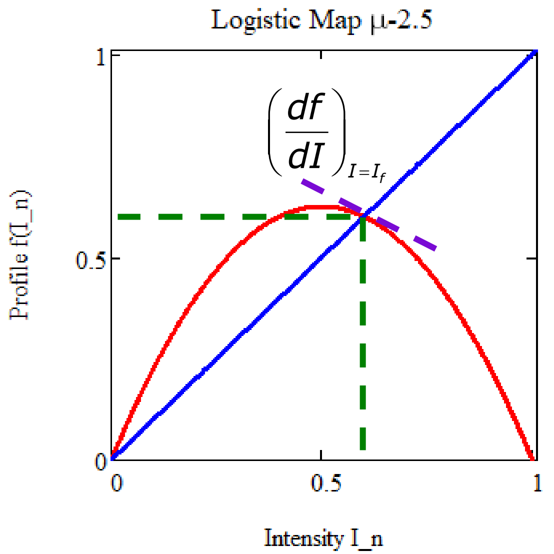
fixpoints "attract" or "repel" (scatter)

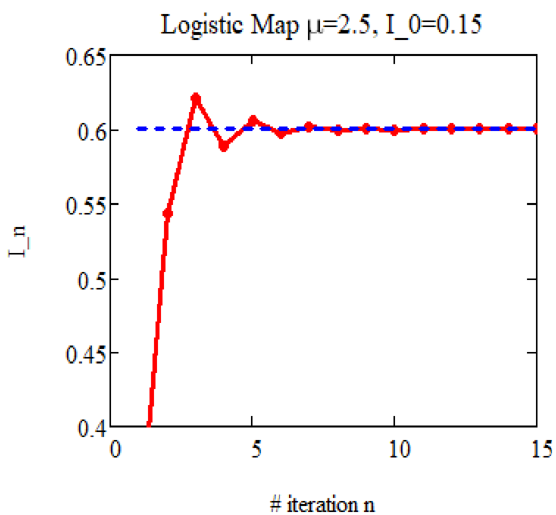
$$\left| \left(\frac{df}{dI} \right)_{I_f} \right| < 1 \quad (I_f = \textit{Attractor})$$

$$\left| \left(\frac{df}{dI} \right)_{I_f} \right| > 1 \quad (I_f = \textit{Repellor, strange attractor})$$

Can you give some plausible geometrical or analytical arguments for this rule?

Logistic Map Features





Profile function *f*, amplification factor $\boldsymbol{\mu}$

$Fixpoints\ I_f : f(I_f) = I_f$ $\quad$ $Trivial\ I_f = 0$

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$$\left|\left(\frac{df}{dI}\right)_{I_f}\right| < 1 \quad (I_f = Attractor)$$

$$\left|\left(\frac{df}{dI}\right)_{I_f}\right| > 1 \quad (I_f = Repellor,\ strange\ attractor)$$

Check behavior by varying initial conditions,
Compare trajectories with ($\boldsymbol{I_0 = I_f} \pm \varepsilon$)
→ Different sensitivity to initial condition.
df > d***I*** → *distance between trajectories grows*

Stability of Complex Systems

Stable Equilibrium

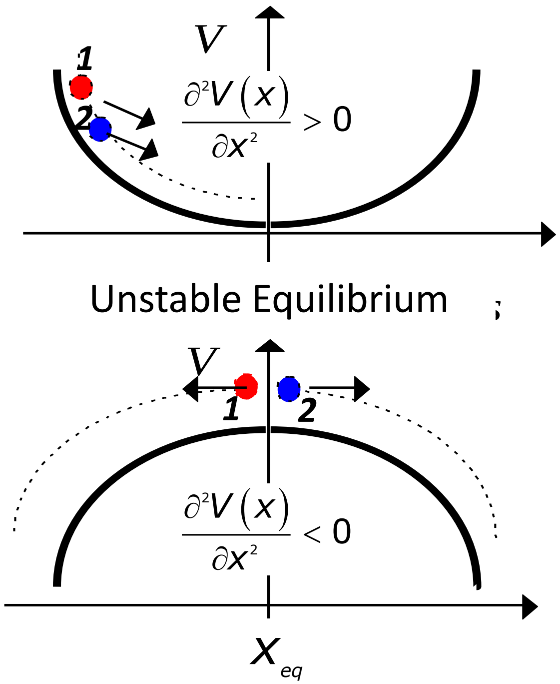


Illustration of potential equilibrium points and trends of neighboring trajectories

What are asymptotic states reached in limit $t, n \rightarrow \infty$?
Can they be reached from any initial conditions?

Specifically: deterministic or chaotic behavior?

→ Need stability criterion,
one-dimensional classical mechanics:

motion driven by a potential $V(x)$

Force equilibrium ←→ $V(x)$=extremum:

$$\left.\frac{\partial V(x)}{\partial x}\right|_{x_{eq}} = 0 \qquad \left.\vec{\nabla} V(\vec{r})\right|_{\vec{r}_{eq}} = \vec{0}$$

Corresponding effects of development of neighboring trajectories:

Converge towards stable equilibrium
Diverge away from unstable equilibrium

Stability of Complex Systems

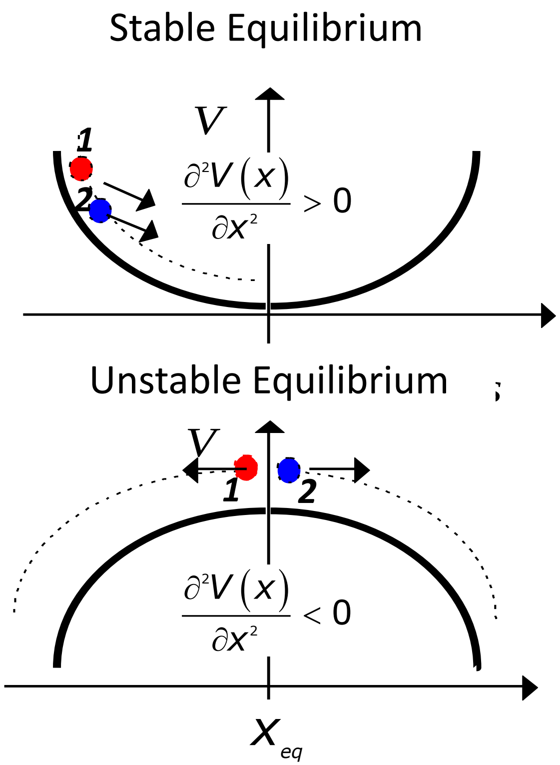


Illustration of potential equilibrium points and trends of neighboring trajectories

Integrate ***1D*** equation of motion *EoM* along ***x*** numerically → *1D* map $\boldsymbol{x_{n+1} = f(x_n)}$

Example: Point particles, mass *m*, force *F*

(Can you write down EoM $\boldsymbol{x}_n = \boldsymbol{x}(t_n)$?)

2 similar initial conditions given ***x*** and $(\boldsymbol{x+\varepsilon})$ small $\varepsilon > 0$.

Step ***n***: trajectories at $f^n(x)$ and $f^n(x+\varepsilon)$

Convergence/divergence ←→ Distance criterion δ

How far apart are initially close trajectories after step ***n?***

$$\delta(\varepsilon, n) := |f^n(x) - f^n(x+\varepsilon)| =: |\varepsilon| \cdot e^{\lambda \cdot n}$$

Legitimate definition of λ, illustrates behavior $n \to \infty$

Lyapunov Stability Criterion

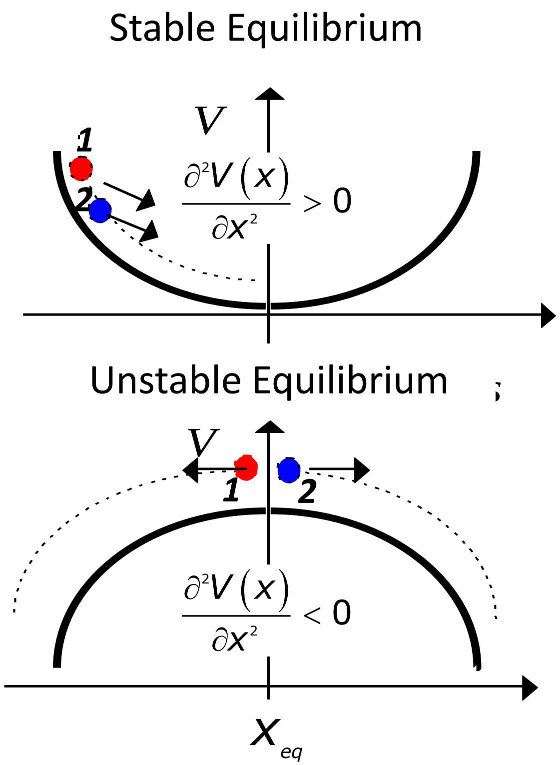


Illustration of potential equilibrium points and trends of neighboring trajectories

Lyapunov exponent:

divergence $\lambda > 0$ Convergence $\lambda < 0$

Large positive exponents indicate extreme sensitivity to initial conditions→ chaotic dynamics

$$\delta(\varepsilon, n) := |f^n(x) - f^n(x+\varepsilon)| =: |\varepsilon| \cdot e^{\lambda \cdot n}$$

$$\rightarrow Ln \left| \left\{ \frac{f^n(x) - f^n(x+\varepsilon)}{\varepsilon} \right\} \right| = \lambda \cdot n$$

Infinitesimal ε

$$\lambda = \frac{1}{n} Ln \left| \frac{df^n(x)}{dx} \right|$$

How to calculate derivative of Implicit function $f^n(x)$?

Lyapunov Exponent

$$\boldsymbol{\lambda} = \frac{1}{n} Ln\left|\frac{df^n(x)}{dx}\right|$$

Implicit function

$$f^n(x) = f(x_{n-1}) = ... = f(f(f(f(x_{n-4}))))....$$

Chain Rule for differentiation:

$$\frac{df^n}{dx} = \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{dx_{n-1}}{dx} = \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{dx_{n-1}}{dx_{n-2}} \cdot \frac{dx_{n-2}}{dx} = ...$$

$$= \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{df(x_{n-2})}{dx} = \frac{df(x_{n-1})}{dx_{n-1}} \cdot \frac{df(x_{n-2})}{dx_{n-2}} \cdot \frac{df(x_{n-3})}{dx_{n-3}} \cdot\cdot\cdot\cdot\cdot \frac{df(x)}{dx}$$

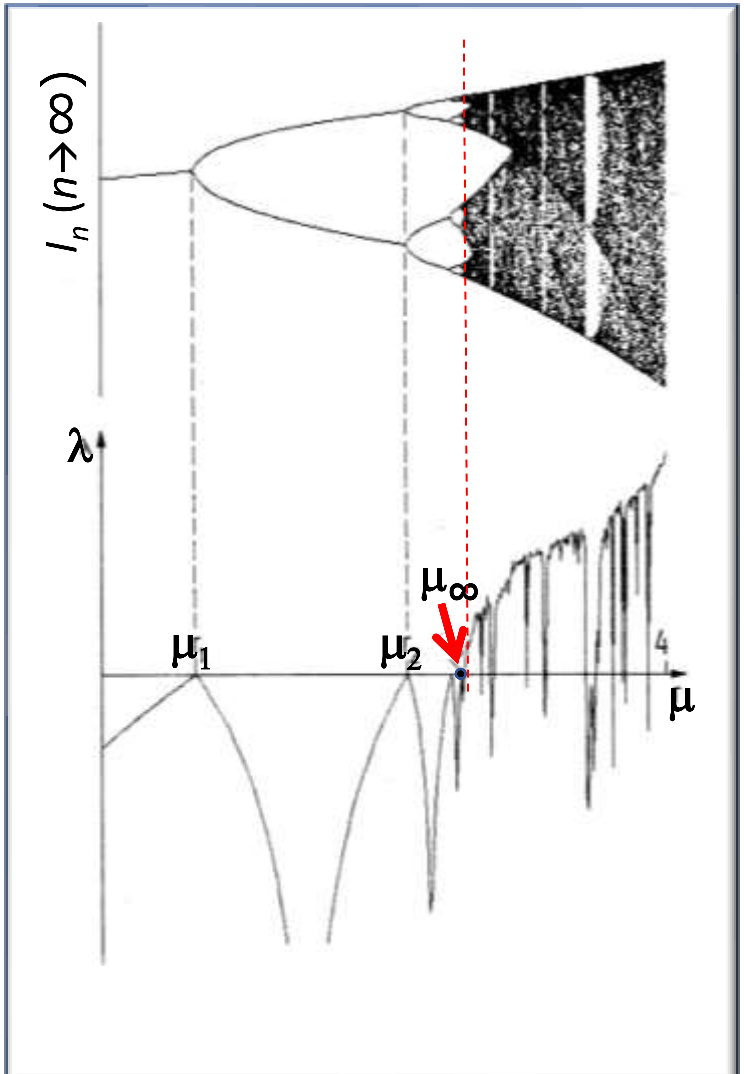
explicit, direct

$$Ln\left|\frac{df^n}{dx}\right| = Ln\prod_{i=0}^{n-1}\left|f'(x_i)\right|_{x_i} = \sum_{i=0}^{n-1} Ln\left|f'(x_i)\right|_{x_i}$$

$$\lambda_n = \frac{1}{n} \cdot \sum_{i=0}^{\mathbf{n}-1} Ln\left|f'(x_i)\right|_{x_i}$$

Large n → test the shape of f at many positions x_i

Lyapunov Exponent = $f(\mu)$



Asymptotic iterates and Lyapunov exponent for the logistic map:

Gain factors μ determine dynamics

$\mu \geq \mu_1$: at least bifurcation

$\mu \geq \mu_2$: at least 2 bifurcations

$\mu \geq \mu_\infty$: λ generally >0, → Chaotic system behavior, small special domains for (relatively) orderly behavior.

Similar :

$f(x) := \mu \cdot x^k \left(1 - x^k\right)^{1/k}$ *and*

$f(x) := \mu(x) \cdot x^k \left(1 - x^k\right)^{1/k}$

Outlook and Conclusions (for our environment)

- ❑ Non-linear dynamics of complex systems can lead to orderly or chaotic behavior, depending on non-linearity → amplification μ for log. map. strength of positive feed back loops.

- ❑ Chaotic dynamics include sudden wild oscillations in system properties at "Tipping Points,"

- ❑ Given an observed non-linear behavior for a specific system (example: Earth albedo), it is possible to estimate a Logistic-Map model amplification parameter $\boldsymbol{\mu}$.

- ❑ Extensions of simple 1D Logistic-Map model include multiple dimensions {x,y} provide understanding of population dynamics (predator-prey)

$$dx/dt = \mu(x,y)\cdot x\cdot\left[1-x\right] \qquad dy/dt = \mu(x,y)\cdot y\cdot\left[1-y\right]$$

- ❑ Earth albedo can change rapidly, leading to tipping points in climate.

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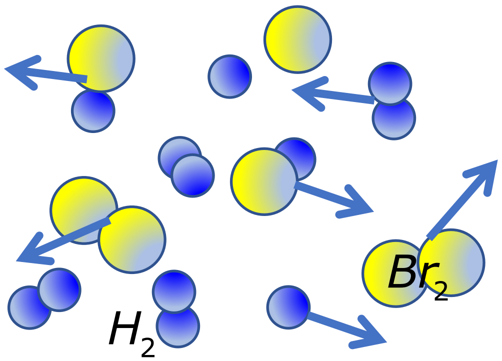
McQuarrie & Simon
Math Chapters
MC B, C, D,

Complex Chemical Kinetics (Example Dissociation)



How do some complex chemical reactions behave? Look at "simple" chemical reactions → often involve several, interrelated steps.

Unlikely to achieve aligned configuration in a collision between H_2 and Br_2

Stoichiometric sum equation

$$H_2 + Br_2 \rightarrow 2HBr$$

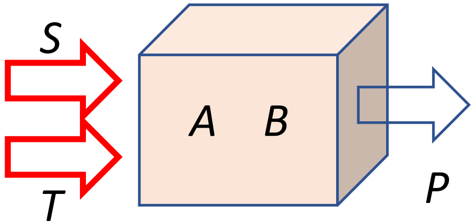
intermediate steps

1.	$Br_2 \rightleftharpoons 2Br$	Br_2 dissociation → atomic Br
2.	$Br + H_2 \rightarrow HBr + H$	*1. HBr* + atomic *H*
3.	$H + Br \rightarrow HBr$	*2. HBr*

Reaction rates for 2. and 3. depend on [atomic *Br*].
Depleting [atomic *Br*] → dissociation of Br_2.
→ ***feed-back*** between the reactions 1 and (2,3) → Le Chatelier Principle
→ Expect complex behavior of coupled chemical reactions (orderly, oscillatory, or chaotic)

Complex Chemical Kinetics (Auto-Catalytic)

Auto-catalytic reaction (like "Brusselator"), following treatment by Kondepudi & Prigogine



External parameters: constant flow of reactants *S* & *T*,

Intrinsic catalysts *A* & *B* →, output product *P*,

Net Reaction

$$S + T \rightarrow P$$

intermediate steps

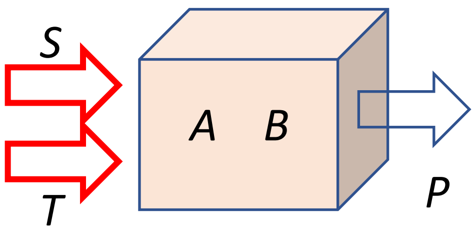
1. $S + T \xrightarrow{k1} A$
2. $S + A \xrightarrow{k2} B$
3. $A + B \xrightarrow{k3} P$

→ 3 reactions coupled through production and consumption of intermediate catalysts *A* and *B*. Constant ("stationary") output *P* desired maintained through constant influx *S and T*

→ ***Set up non-equilibrium rate equations, look for stationary concentrations.***

Complex Chemical Kinetics (Auto-Catalytic)

Auto-catalytic reaction



$$S + T \rightarrow P \quad \Rightarrow \quad \begin{cases} 1.\ S + T \xrightarrow{k1} A \\ 2.\ S + A \xrightarrow{k2} B \\ 3.\ A + B \xrightarrow{k3} P \end{cases}$$

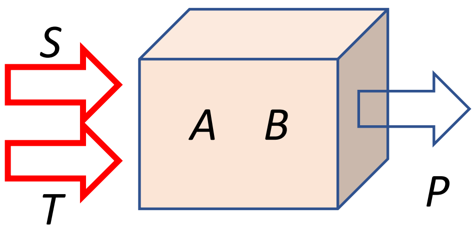
$$Define\ concentrations\ \vec{X} = \begin{pmatrix} [A] \\ [B] \end{pmatrix}, t - dep.\ rates\ \vec{Z} = \frac{d}{dt}\begin{pmatrix} [A] \\ [B] \end{pmatrix}$$

Rate equations,
Constant external input
flows [S], [*T*]

$$\begin{cases} \frac{d}{dt}X_1 = k_1 \cdot [S] \cdot [T] - k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = Z_1\left(\vec{X}, [S], [T]\right) \\ \\ \frac{d}{dt}X_2 = k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = Z_2\left(\vec{X}, [S], [T]\right) \end{cases}$$

Complex Chemical Kinetics (Auto-Catalytic)

Auto-catalytic reaction



$$S + T \rightarrow P \quad \Rightarrow \quad \begin{cases} 1.\ S + T \xrightarrow{k1} A \\ 2.\ S + A \xrightarrow{k2} B \\ 3.\ A + B \xrightarrow{k3} P \end{cases}$$

Stationary concentration of B: $dX_2/dt = k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2$

$$\frac{d}{dt}[B] = \frac{d}{dt}X_2 = 0 \quad \Rightarrow \quad k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = 0$$

$$k_2 \cdot [S] \cdot X_1 = k_3 \cdot X_1 \cdot X_2 \rightarrow \boxed{X_2 = \frac{k_2}{k_3} \cdot [S]}$$

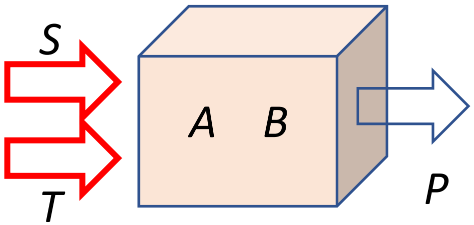
Stationary concentration of A: $dX_1/dt = k_1 \cdot [S] \cdot [T] - k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2$

$$\frac{d}{dt}[A] = \frac{d}{dt}X_1 = 0 \quad \Rightarrow \quad k_1 \cdot [S] \cdot [T] - k_2 \cdot [S] \cdot X_1 - k_3 \cdot X_1 \cdot X_2 = 0$$

$$k_1 \cdot [S] \cdot [T] = 2k_2 \cdot [S] \cdot X_1 \rightarrow \boxed{X_1 = \frac{k_1}{2k_2} \cdot [T]}$$

Complex Chemical Kinetics (Auto-Catalytic Rxns)

Auto-catalytic reaction



$$S + T \to P \quad \Rightarrow \quad \begin{cases} 1.\ S + T \xrightarrow{k1} A \\ 2.\ S + A \xrightarrow{k2} B \\ 3.\ A + B \xrightarrow{k3} P \end{cases}$$

Stationary state concentrations

$$[A]_s = X_{1s} = \frac{k_1}{2k_2} \cdot [T]; \quad [B]_s = X_{2s} = \frac{k_2}{k_3} \cdot [S]$$

Stationary state concentrations: At given [*S*] and [*T*], intermediates *A* and *B*, and product *P* reach extreme values in time. But is mode of operation stable or unstable?

Check how small variations in extreme values $\boldsymbol{X_{1s}}, \boldsymbol{X_{2s}}$ change with time:

$$X_{ns} \to (X_{ns} + \delta X_{ns}) \xrightarrow{Rate\ Eqs} \frac{d}{dt}(X_{ns} + \delta X_{ns})_t \to \delta X_{ns}(t);\ n = 1,2$$

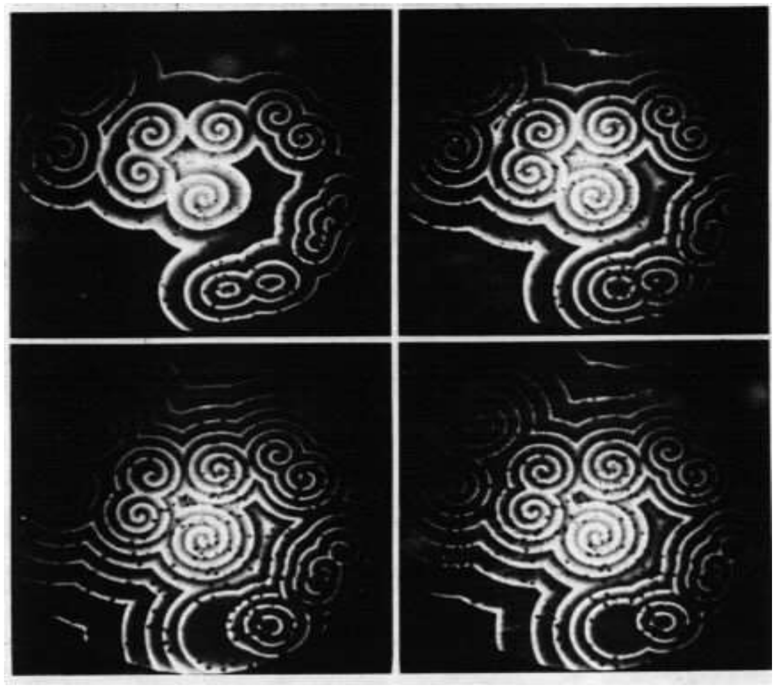
For stable ops, $\delta X_{ns}(t)$ *should vanish* $t \to \infty$

Cooperative Belousov-Zhabotinski (BZ) Reaction

Oxidation of malonic acid with cerium bromate, *$CeBr_3$* (*Kondepudi&Prigogine Ch. 19*)

$$2BrO_3^- + 3CH_2(COOH)_2 + 2H^+ \rightarrow 2BrCH(COOH)_2 + 3CO_2 + 4H_2O$$

Produces colored traveling wave patterns on surface of reaction vessel.

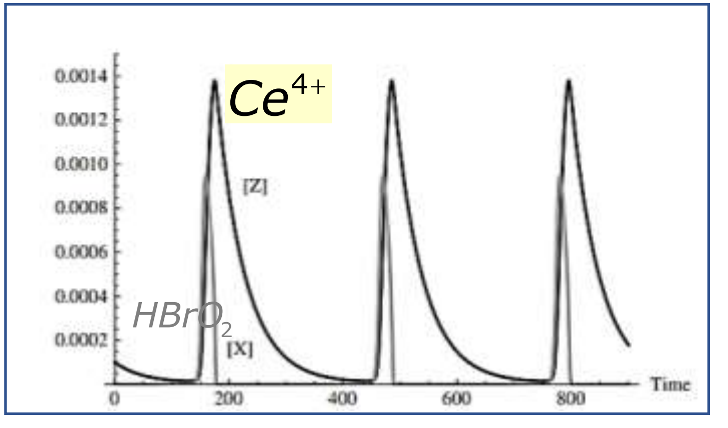


Ce catalyst, [*Ce*]=const., but oscillations between *Ce^{3+}* and *Ce^{4+}*, → alternating colors.

Intermediate reaction step

$$BrO_2 + Ce^{3+} + H^+ \rightarrow HBrO_2 + Ce^{4+}$$

Similar oscillations: Lotka-Volterra



Relevant Intro Literature

- The New Physics, Paul Davis (Editor), Cambridge University Press New York, 1989.,Wiley-Interscience Publ., New York 1998
- A. Babloyantz, Molecules, Dynamics, and Life; An Introduction to Self-Organization of Matter, Wiley-Interscience Publ., New York 1986
- H. O. Peitgen, H. Jürgens, D. Saupe, Chaos and Fractals – New Frontiers of Science, Springer Verlag New York, 1992.
- G.L. Baker and J.P. Gollub, Chaotic Dynamics, an Introduction, Cambridge University Press, Cambridge 1996.
- C. Beck and F. Schlögl, Thermodynamics of chaotic systems, Cambridge University Press, Cambridge 1993.
- F. Scheck: Mechanics, From Newton's Laws to Deterministic Chaos (Ch. 6.4), Springer Verlag Berlin 1990.
- R. Dawkins: The Blind Watchmaker, W.W. Norton&Co., New York 1986