Mathematics and Pattern Formation in Chemistry and Biology

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Web-Page for further information:

http://www.tbi.univie.ac.at/~pks

1. Equilibrium structures and dissipative patterns
2. Spatio-temporal patterns in chemical reactions
3. Patterns in development
4. Genetic and metabolic networks
5. Patterns in neurobiology

1. **Equilibrium structures and dissipative patterns**
2. Spatio-temporal patterns in chemical reactions
3. Patterns in development
4. Genetic and metabolic networks
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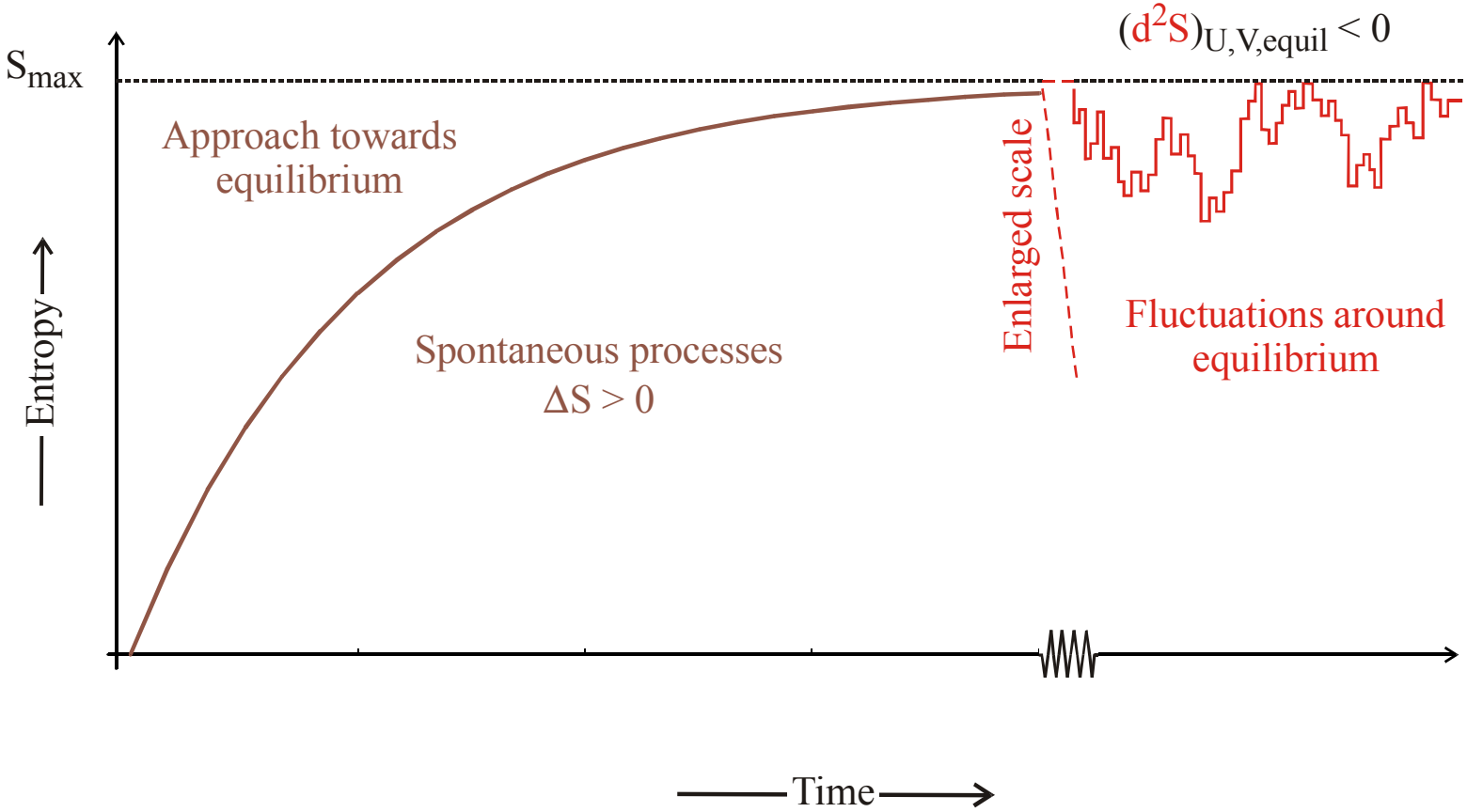
Equilibrium thermodynamics is based on two major statements:

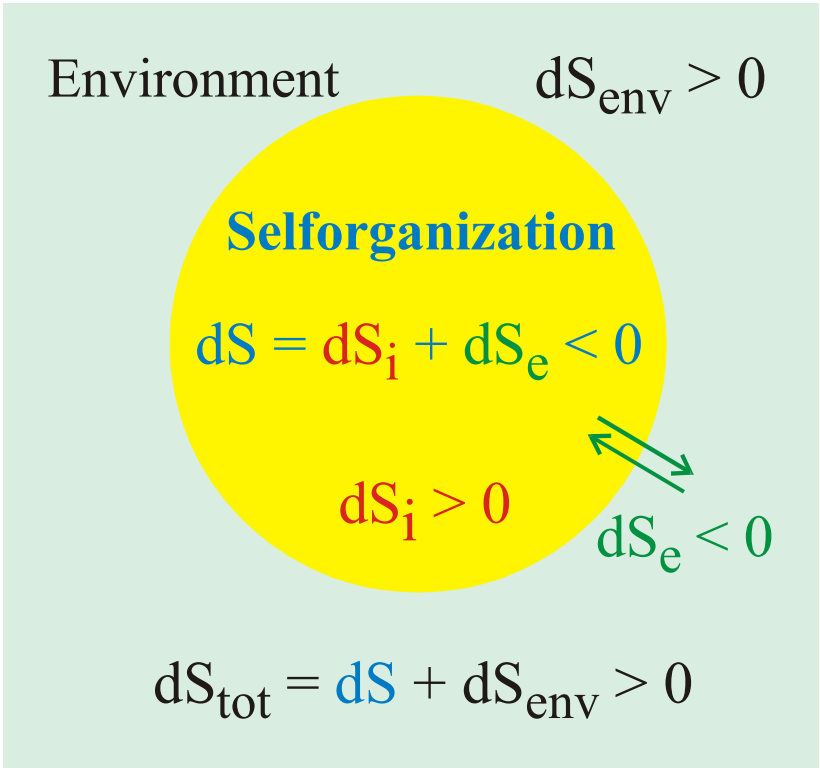
1. *The energy of the universe is a constant (first law).*
2. *The entropy of the universe never decreases (second law).*

Carnot, Mayer, Joule, Helmholtz, Clausius, ……

D.Jou, J.Casas-Vázquez, G.Lebon, *Extended Irreversible Thermodynamics*, 1996



Entropy and fluctuations at equilibrium

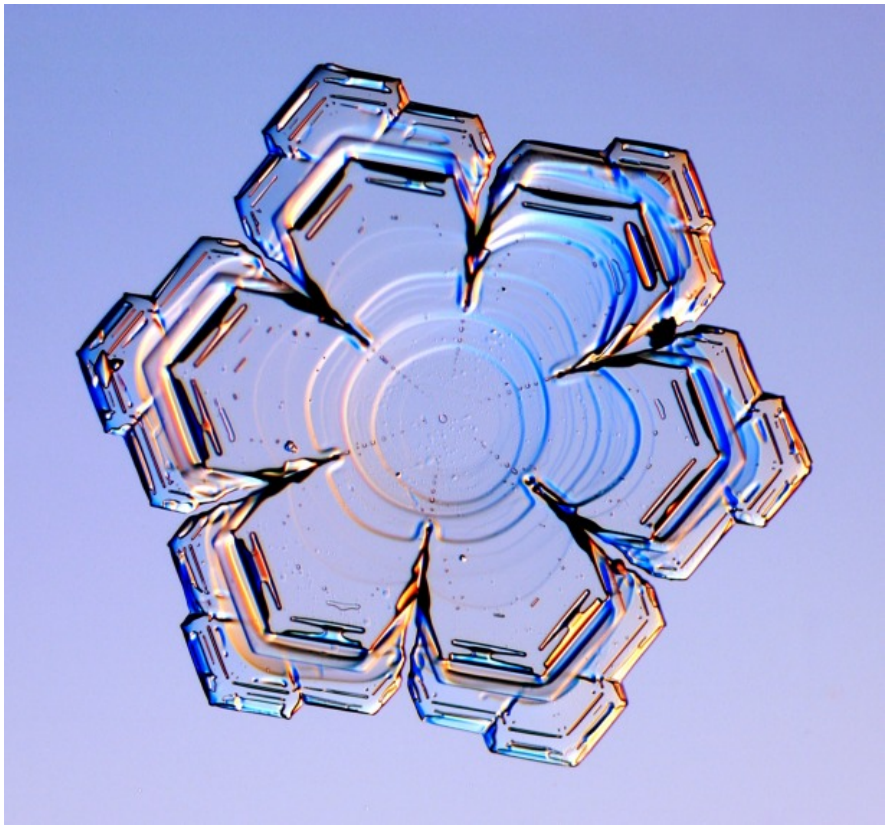


Entropy is equivalent to *disorder*. Hence there is no spontaneous creation of order at equilibrium.

Self-organization is spontaneous creation of order.

Self-organization requires export of entropy to an environment which is almost always tantamount to an *energy flux* or *transport of matter* in an *open system*.

Entropy production and self-organization in open systems

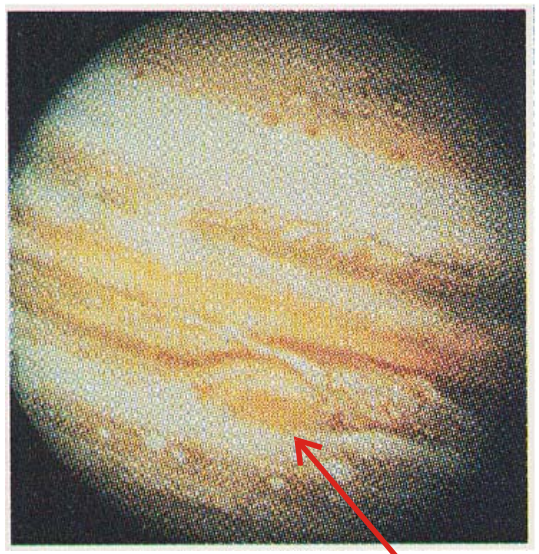


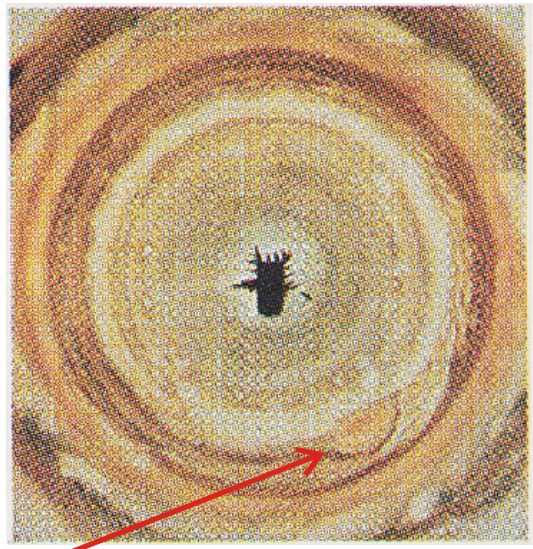
Snowflakes as examples of equilibrium structures that do not require energy for their maintenance

Five examples of self-organization and spontaneous creation of order

- *Hydrodynamic pattern formation in the atmosphere of Jupiter*
- *Pattern formation in heated fluids*
- *Pattern formation in chemical reactions*
- *Morphogenesis in the development of embryos*
- *Patterns in neurobiology*

Examples of self-organization and pattern formation

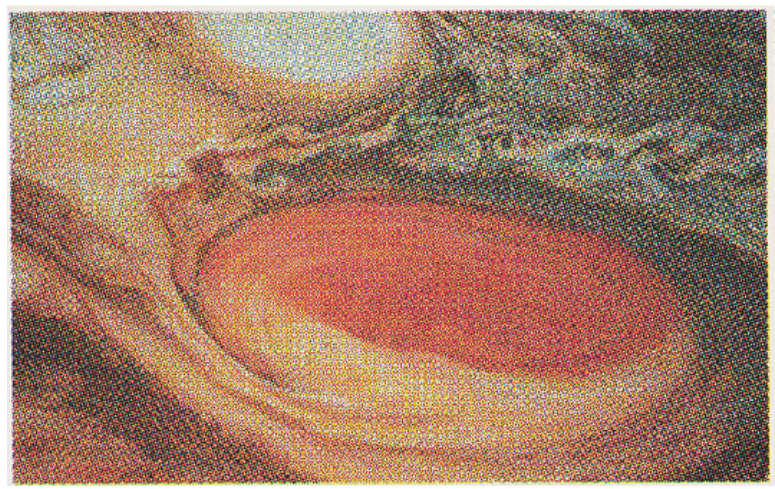




View from south pole

South pole

Red spot



Jupiter: Observation of the gigantic vortex

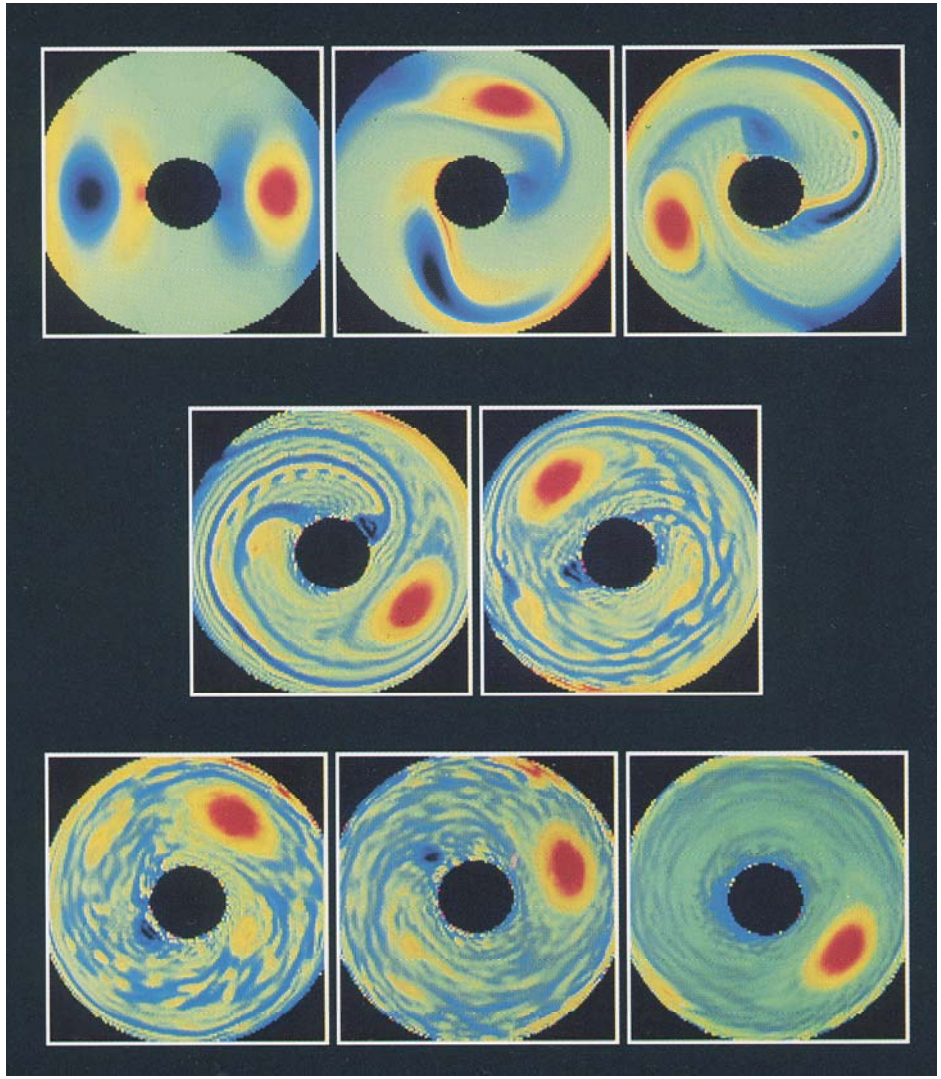
Picture taken from James Gleick, *Chaos*. Penguin Books, New York, 1988

Computer simulation of the gigantic vortex on Jupiter

View from south pole

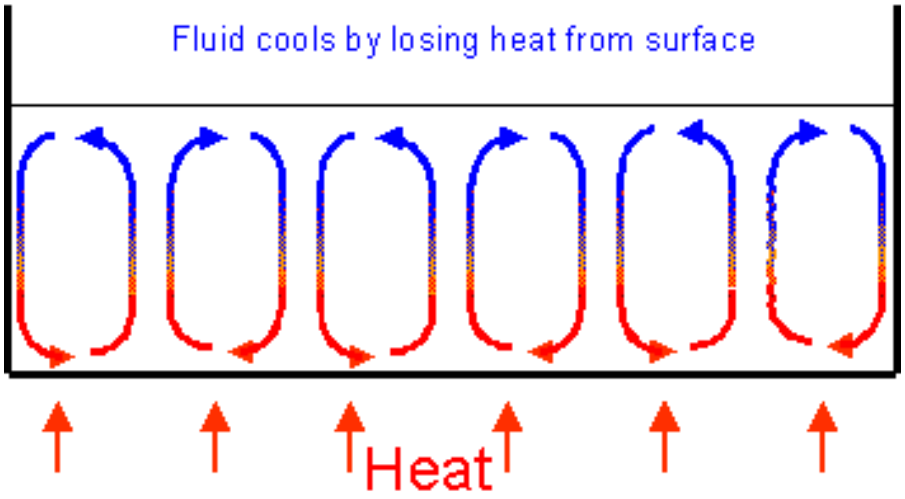
Particles turning counterclockwise

Particles turning clockwise

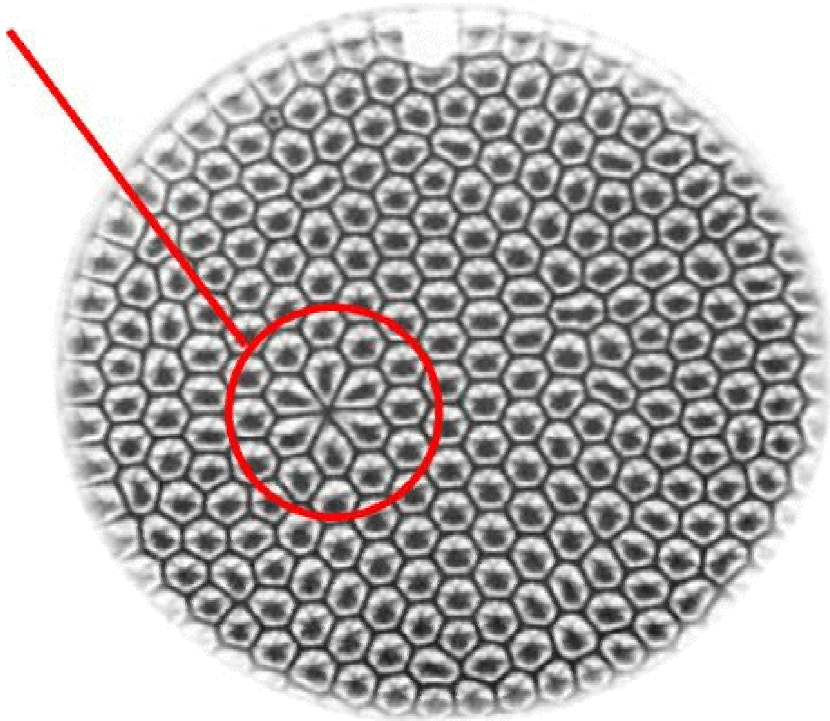


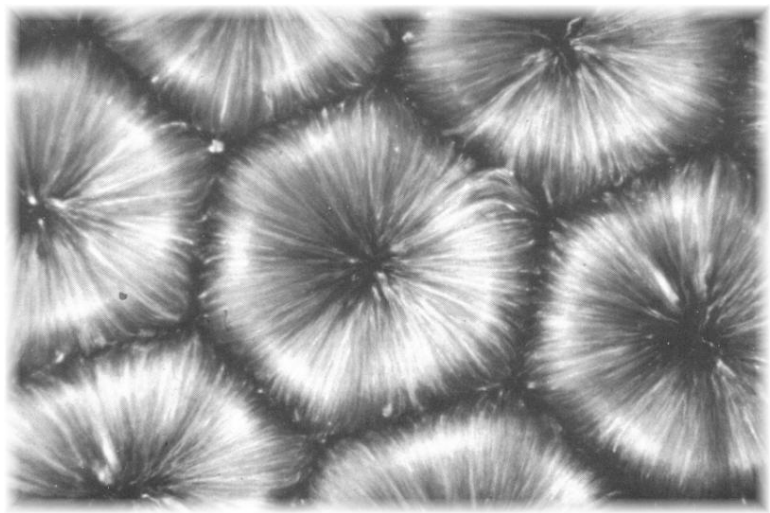
Jupiter: Computer simulation of the giant vortex

Philip Marcus, 1980. Picture taken from James Gleick, *Chaos*. Penguin Books, New York, 1988

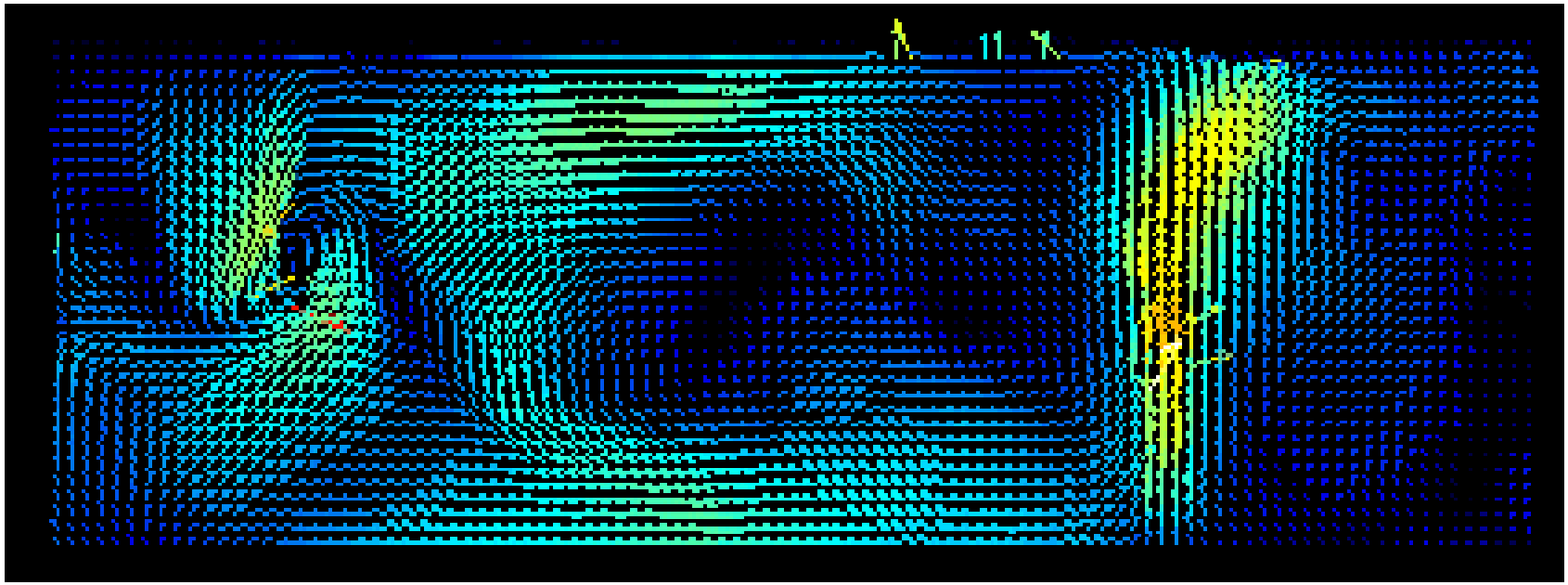


Convection cell
Warm, low density fluid rises
Cool, high density fluid sinks

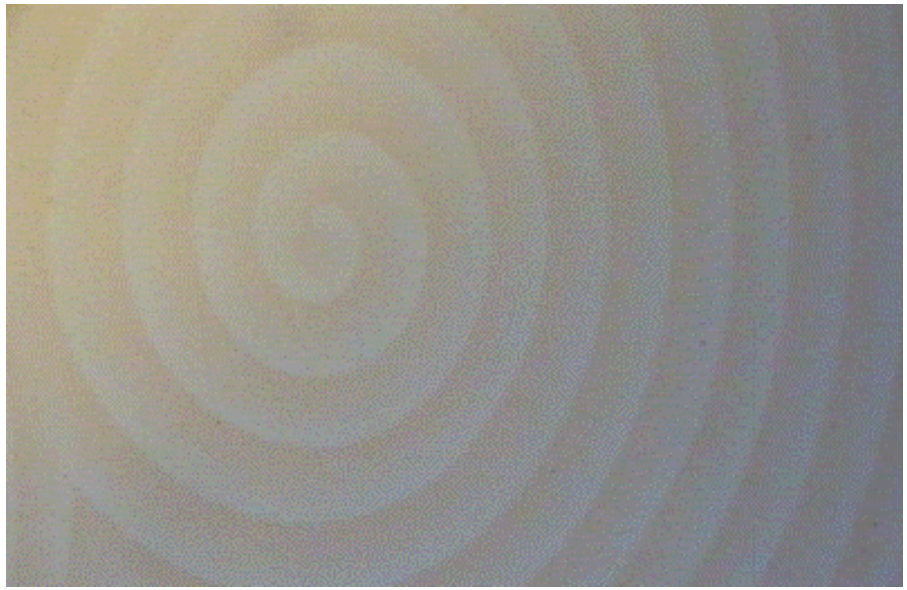




Rayleigh-Benard convention cells in heated fluids



Alberto Petracci. Particle image velocimetry (PIV) measurement of convective flow in a Raleigh-Benard convection cell of dimension 60×60×20 mm



Spatio-temporal pattern in the
Belousov-Zhabotinskii reaction

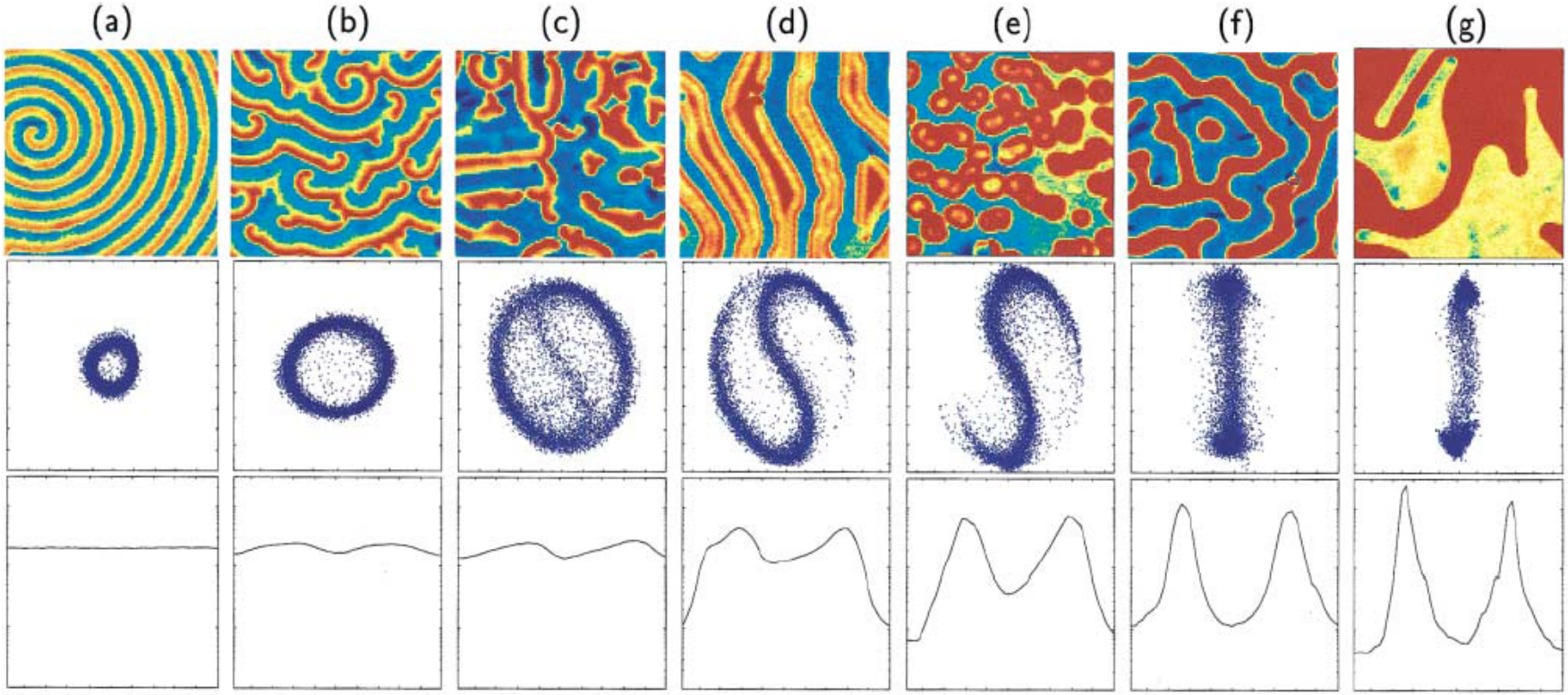
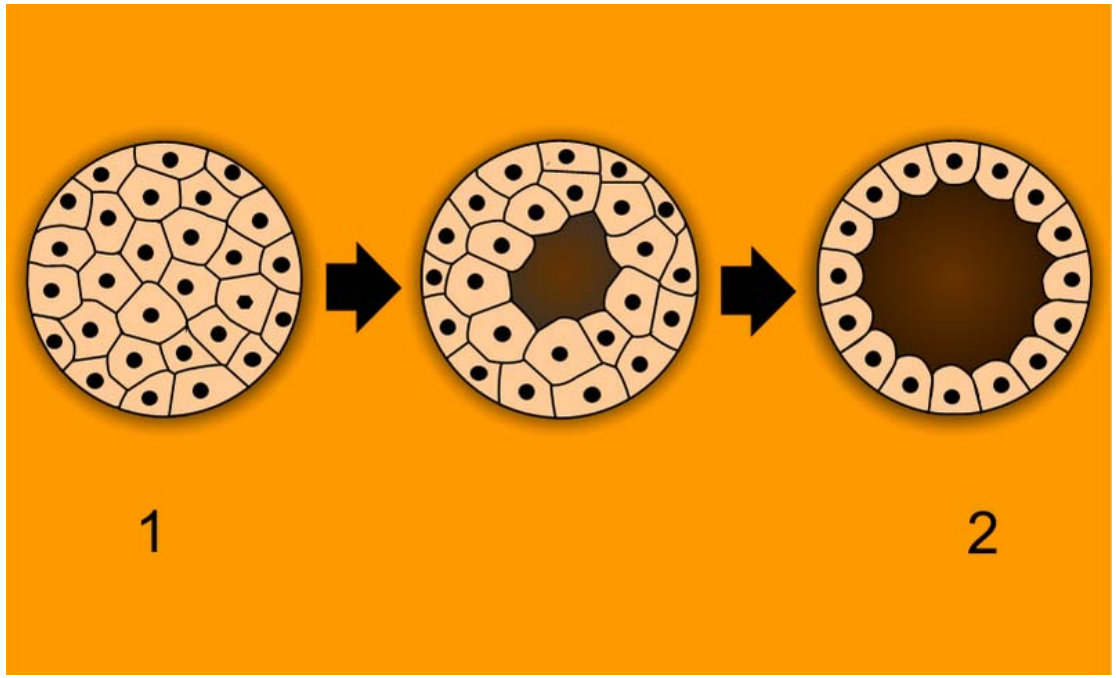


FIG. 2 (color). (top row) Reactor images (9×9 mm^2) of different observed patterns, presented using a rainbow (false) color map: (a) unforced rotating spiral wave, (b) rotating spiral wave, (c) mixed rotating spiral and standing wave pattern, (d)–(g) qualitatively different standing wave patterns. Patterns (b)–(g) exhibit a 2:1 resonance in the temporal power spectrum of the pattern. (middle row) The complex Fourier amplitude $\mathbf{a}$ for each image: the abscissa is Re($\mathbf{a}$); the ordinate is Im($\mathbf{a}$). Each point in the complex plane corresponds to the temporal Fourier amplitude $\mathbf{a}$ of a pixel in the image after frequency demodulation at $f/2$. (bottom row) Histograms of phase angles of all the pixels in each image; the abscissa range is $[0, 2\pi]$ radians and the ordinate range is arbitrary. Chemical conditions are given in [9]. For each pattern the parameter values of f(Hz) and γ^2(W/m^2) are, respectively, (a) 0, 0; (b) 0.1000, 119; (c) 0.0625, 214; (d) 0.0556, 248; (e) 0.0417, 358; (f) 0.0455, 386; (g) 0.0385, 412, and correspond to the circled points in Fig. 1.

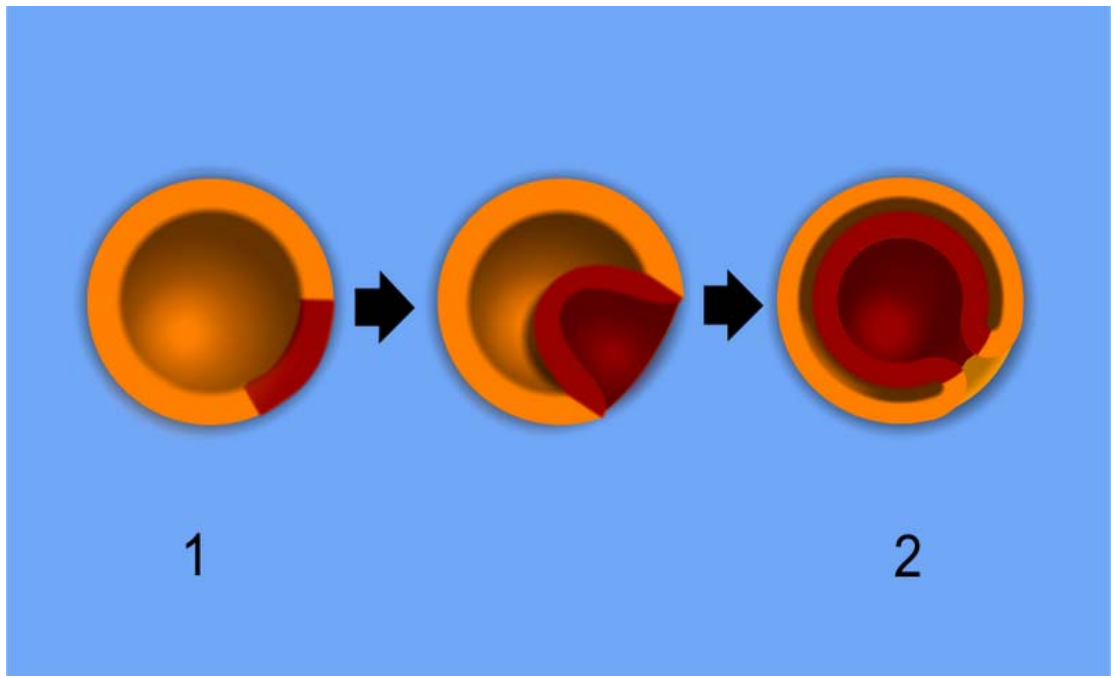
Pattern formation in the Belousov-Zhabotinskii reaction

Anna L. Lin, Matthias Bertram, Karl Martinez, and Harry L. Swinney, *Phys.Rev.Letters* **84**, 4240 (2000)

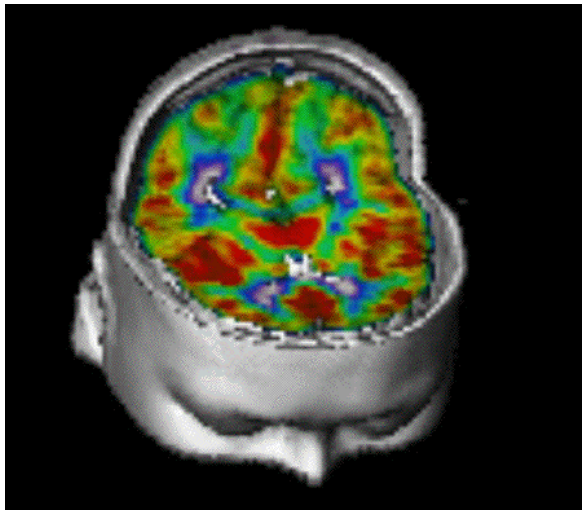
blastulation

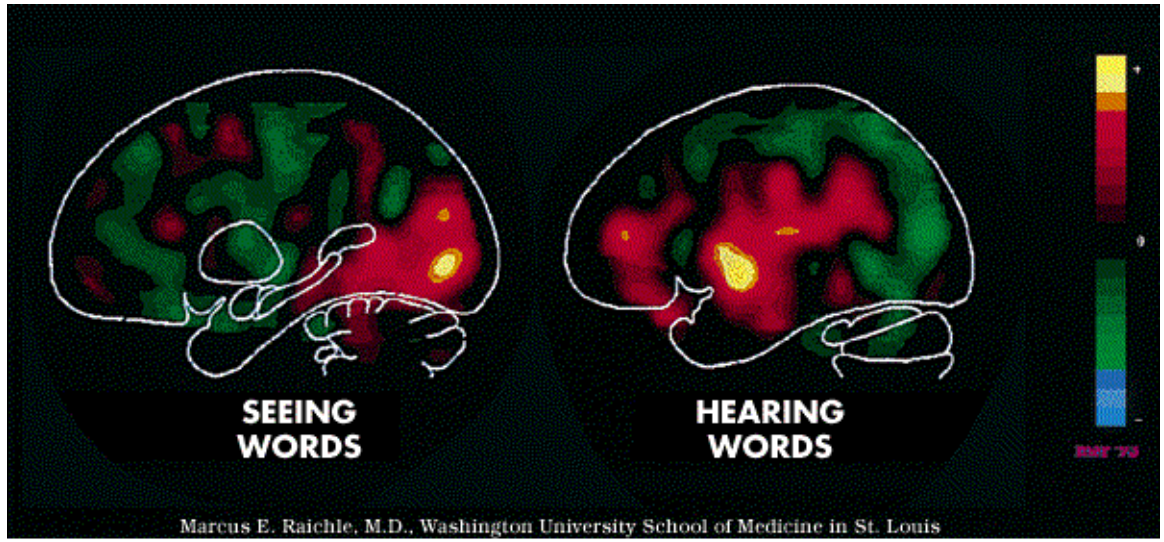


gastrulation



Pattern formation in
animal development

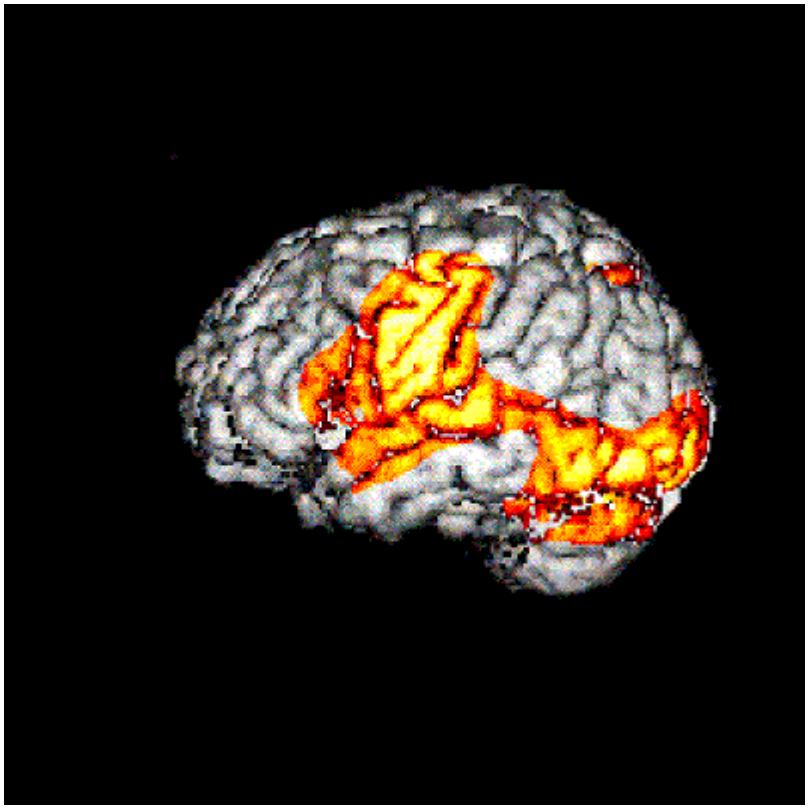




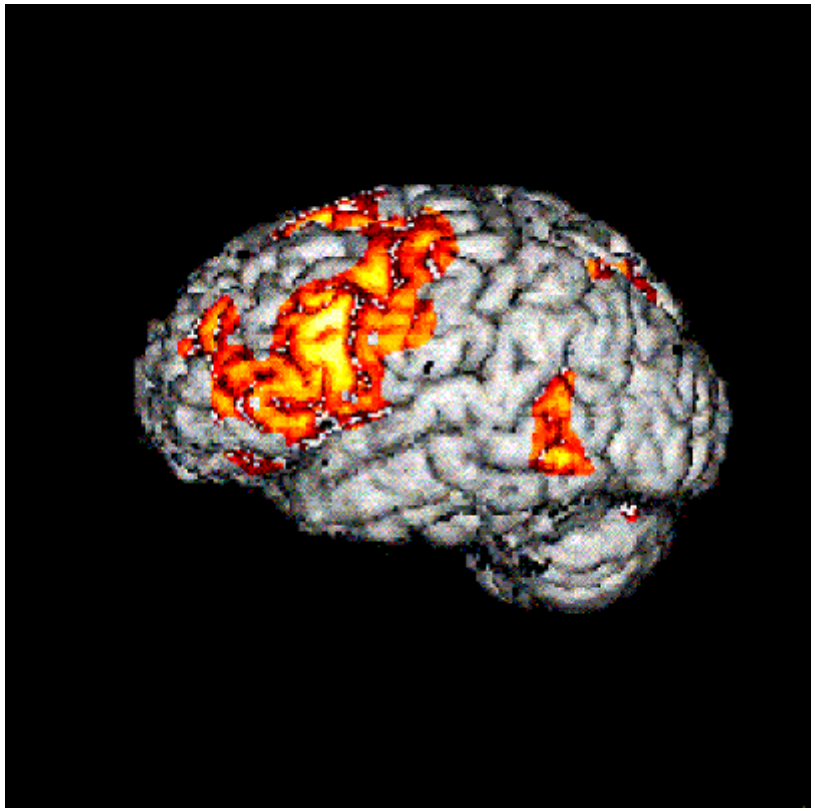
The PET scan on the left shows two areas of the brain (red and yellow) that become particularly active when volunteers read words on a video screen: the primary visual cortex and an additional part of the visual system, both in the back of the left hemisphere. Other brain regions become especially active when subjects hear words through ear-phones, as seen in the PET scan on the right.

Specific pattern formation in the brain correlates with certain activities.

Pictures from the web-page of the Neurobiology Research Unit, Rigshospitalet, Copenhagen, Denmark



reading aloud



silent generation of words

Brain activity relative to the resting state

Pictures from the web-page of the Neurobiology Research Unit, Rigshospitalet, Copenhagen, Denmark

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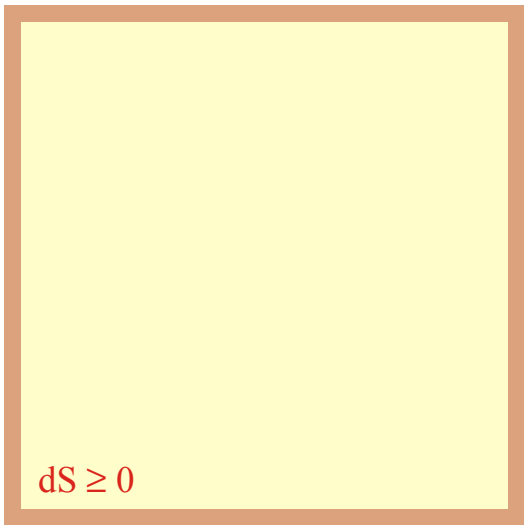
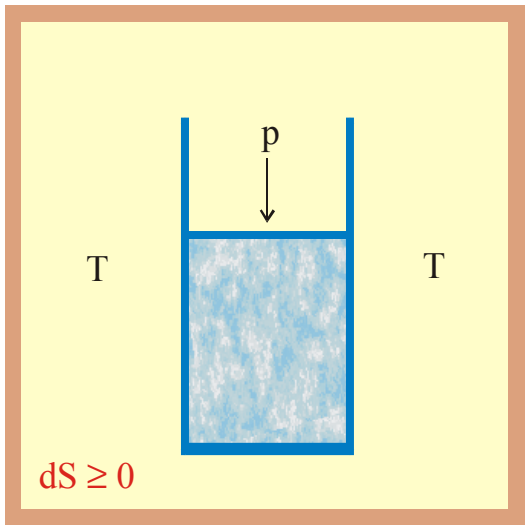


Isolated system

U = const., V = const.,

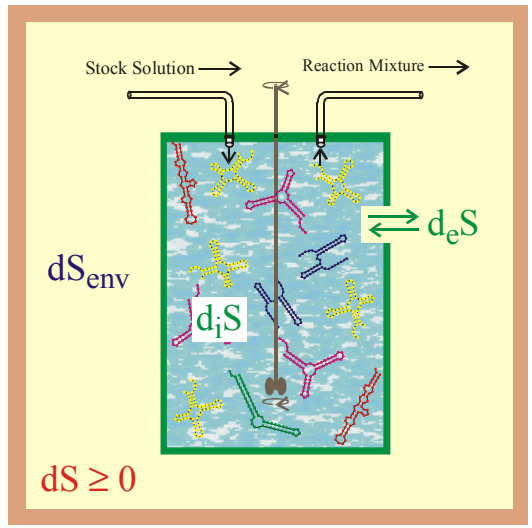
dS ≥ 0



Closed system

T = const., p = const.,

dG = dU-pdV-TdS ≤ 0



Open system

$dS = dS_{env} + dS \geq 0$

$dS = d_iS + d_eS$

$d_iS \geq 0$

Entropy changes in different thermodynamic systems

$* \rightarrow A$

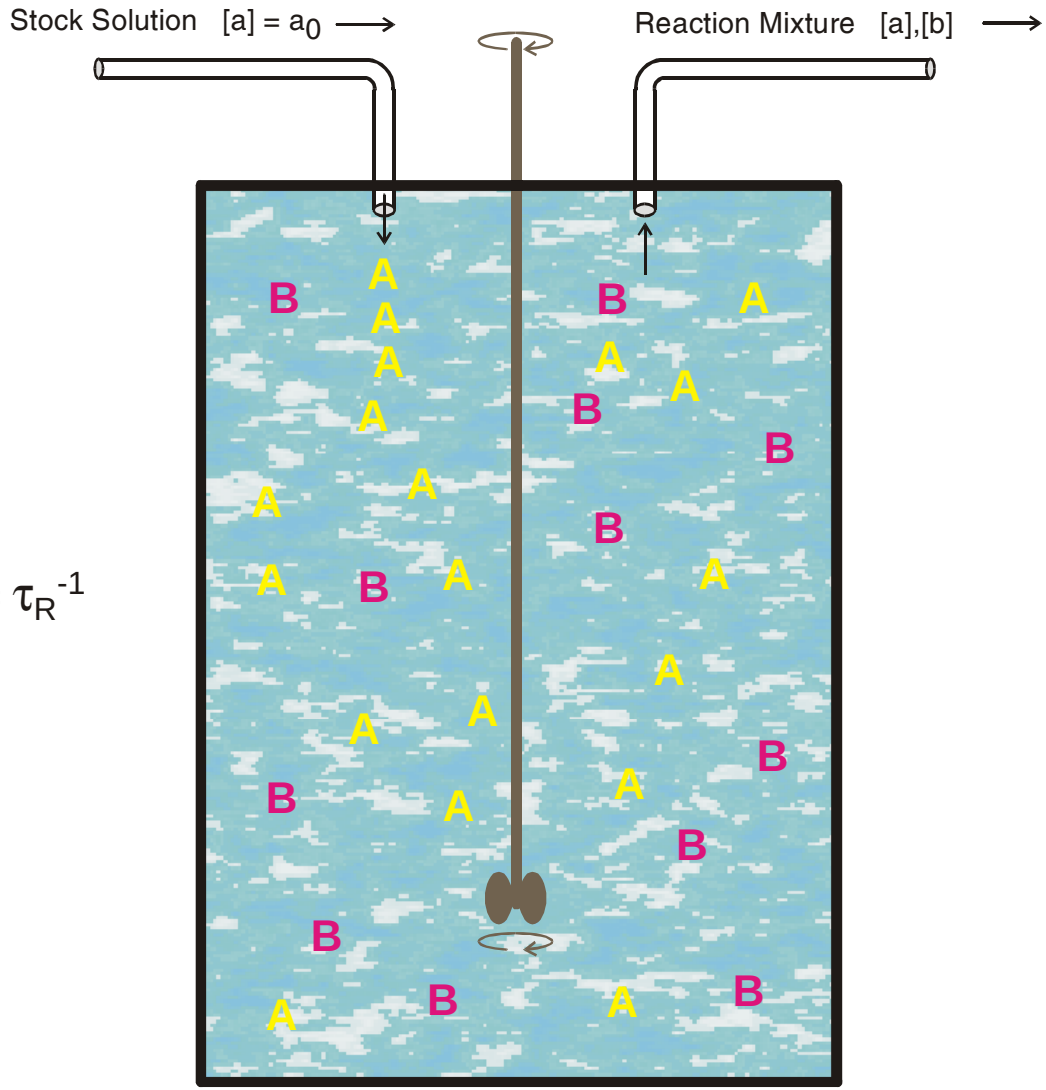
$A \rightarrow B$

$A \rightarrow \varnothing$

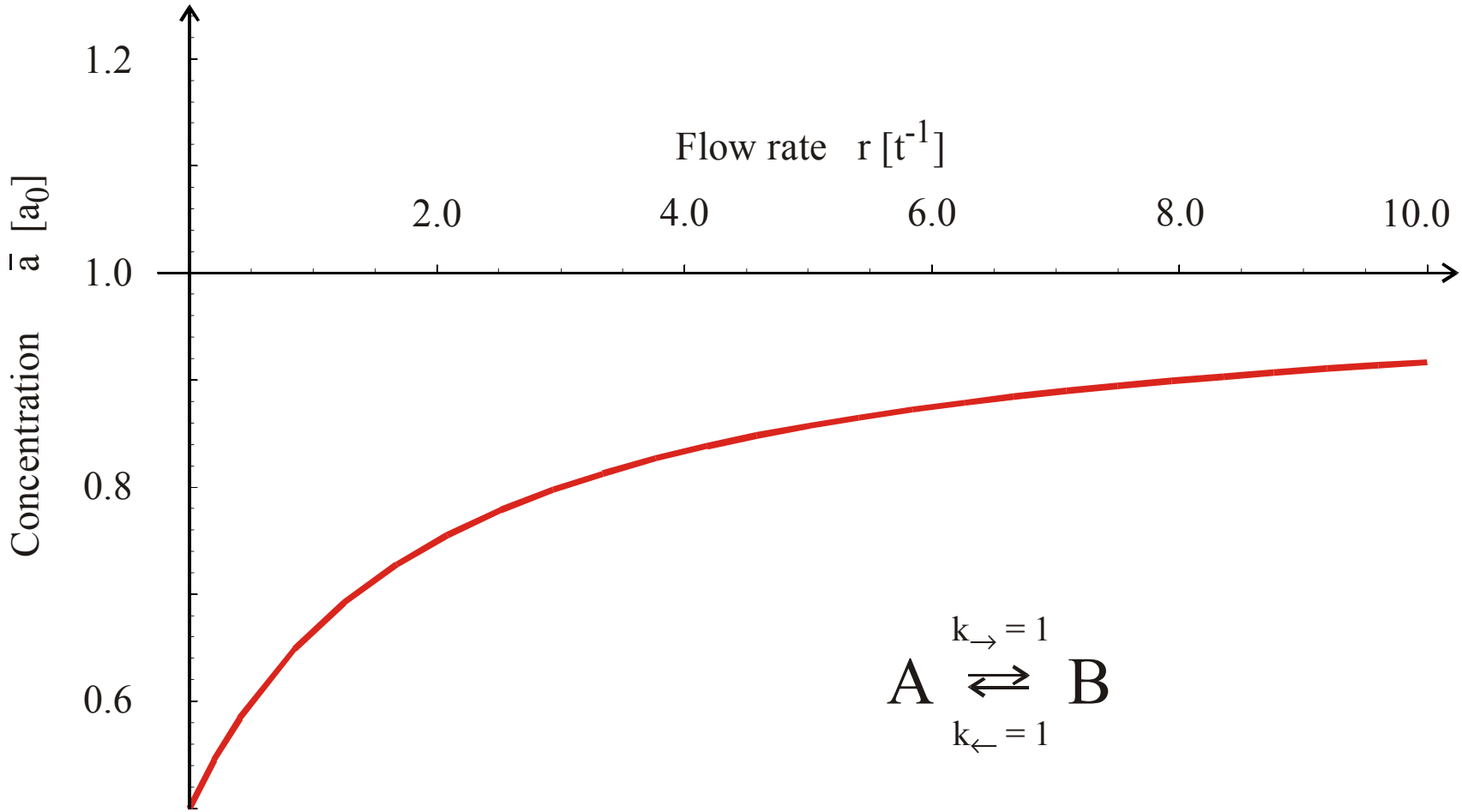
$B \rightarrow A$

$B \rightarrow \varnothing$

Flow rate $r = \tau_R^{-1}$



Reactions in the continuously stirred tank reactor (CSTR)



Reversible first order reaction in the flow reactor

$$* \xrightarrow{r} \mathbf{A}$$

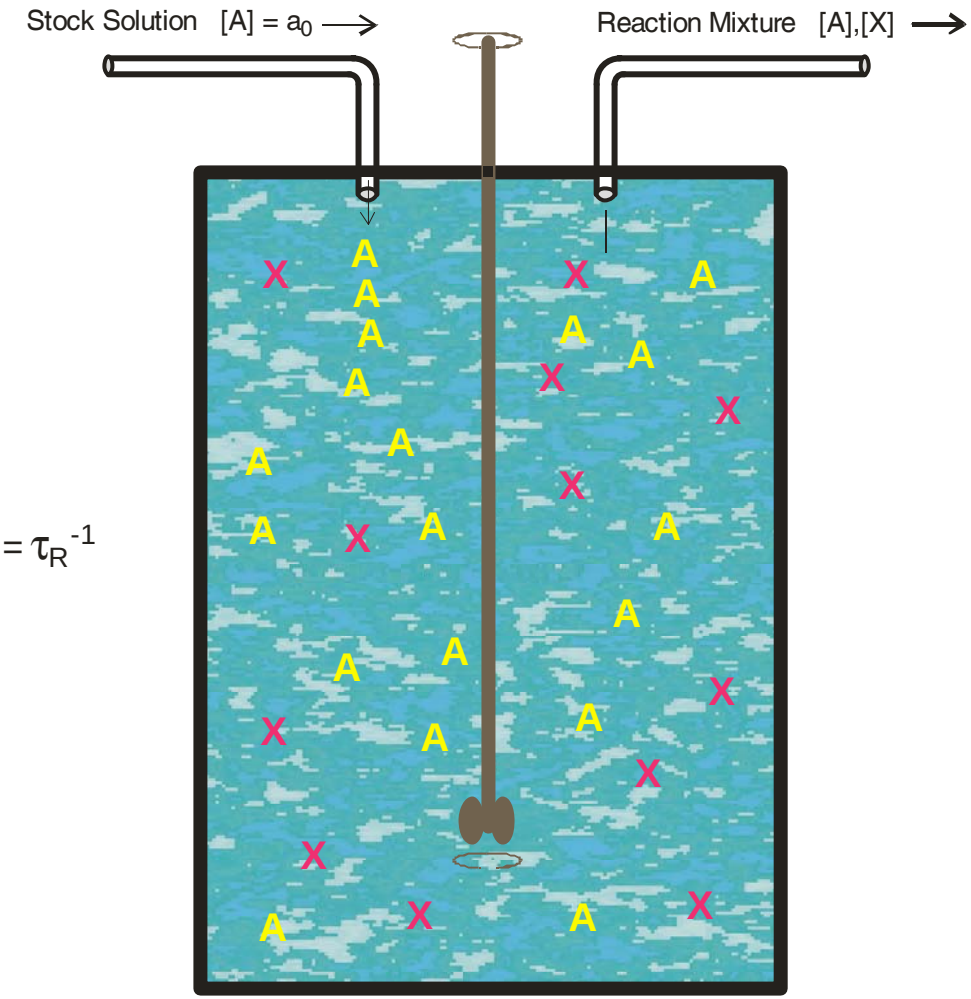
$$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathbf{X}$$

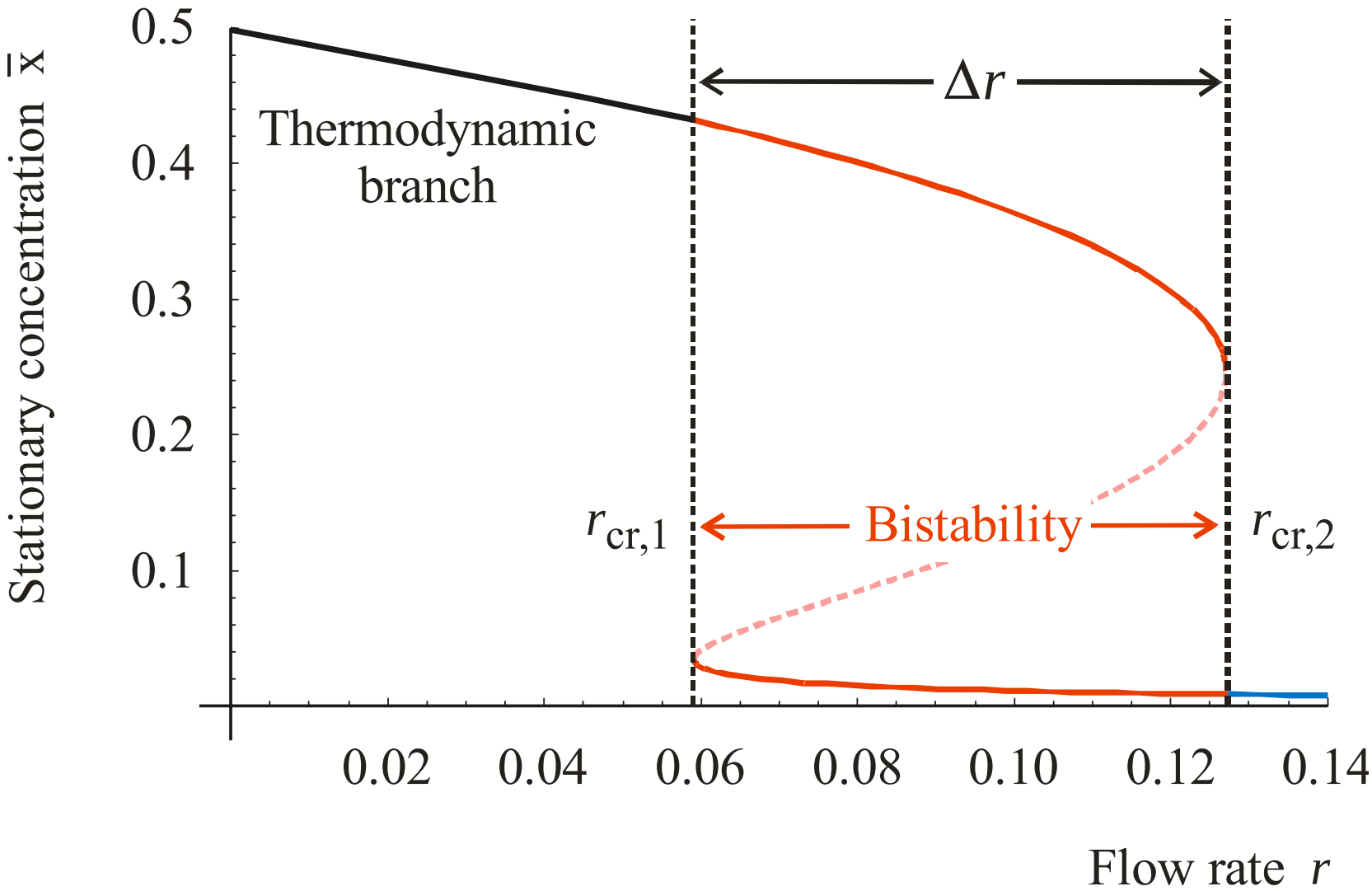
$$\mathbf{A} + 2\,\mathbf{X} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} 3\mathbf{X}$$

$$\mathbf{A} \xrightarrow{r} 0$$

$$\mathbf{X} \xrightarrow{r} 0$$

Flow rate $r = \tau_R^{-1}$




Stationary concentration $\bar{x}$
0.5
0.4
0.3
0.2
0.1
Thermodynamic branch
Δr
$r_{cr,1}$
Bistability
$r_{cr,2}$
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Flow rate r

$$* \xrightarrow{r} \mathbf{A}$$

$$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathbf{X}$$

$$\mathbf{A} + 2\,\mathbf{X} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} 3\mathbf{X}$$

$$\mathbf{A} \xrightarrow{r} 0$$

$$\mathbf{X} \xrightarrow{r} 0$$

Kinetic differential equations:

$$\frac{\mathrm{d[A]}}{\mathrm{dt}} = \frac{\mathrm{d}a}{\mathrm{dt}} = r\,(a_0 - a) - (k_1 + k_3 x^2)\,a + (k_2 + k_4 x^2)\,x$$

$$\frac{\mathrm{d[X]}}{\mathrm{dt}} = \frac{\mathrm{d}x}{\mathrm{dt}} = -\,r\,x + (k_1 + k_3 x^2)\,a - (k_2 + k_4 x^2)\,x$$

$$* \xrightarrow{r} \mathbf{A}$$

$$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftarrows}} \mathbf{X}$$

$$\mathbf{A} + 2\,\mathbf{X} \underset{k_4}{\overset{k_3}{\rightleftarrows}} 3\mathbf{X}$$

$$\mathbf{A} \xrightarrow{r} 0$$

$$\mathbf{X} \xrightarrow{r} 0$$

Kinetic differential equations:

$$\frac{\mathrm{d[A]}}{\mathrm{dt}} = \frac{\mathrm{d}a}{\mathrm{dt}} = r\,(a_0 - a) - (k_1 + k_3 x^2)\,a + (k_2 + k_4 x^2)\,x$$

$$\frac{\mathrm{d[X]}}{\mathrm{dt}} = \frac{\mathrm{d}x}{\mathrm{dt}} = -\,r\,x + (k_1 + k_3 x^2)\,a - (k_2 + k_4 x^2)\,x$$

Steady states:

$$\bar{x}^3 (k_3 + k_4) - \bar{x}^2 k_3 a_0 + \bar{x}(k_1 + k_2 + r) - k_1 a_0 = 0$$

$$* \xrightarrow{r} \mathbf{A}$$

Kinetic differential equations:

$$\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}t} = \frac{\mathrm{d}a}{\mathrm{d}t} = r\,(a_0 - a) - (k_1 + k_3 x^2)\,a + (k_2 + k_4 x^2)\,x$$

$$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathbf{X}$$

$$\frac{\mathrm{d}[\mathrm{X}]}{\mathrm{d}t} = \frac{\mathrm{d}x}{\mathrm{d}t} = -\,r\,x + (k_1 + k_3 x^2)\,a - (k_2 + k_4 x^2)\,x$$

$$\mathbf{A} + 2\,\mathbf{X} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} 3\mathbf{X}$$

Steady states:

$$\bar{x}^3 (k_3 + k_4) - \bar{x}^2 k_3 a_0 + \bar{x}(k_1 + k_2 + r) - k_1 a_0 = 0$$

$$\mathbf{A} \xrightarrow{r} 0$$

$$k_1 = k_2 = \alpha,\ k_3 = k_4 = 1: \quad 2\bar{x}^3 - \bar{x}^2 a_0 + \bar{x}(r + 2\alpha) - \alpha a_0 = 0$$

$$\mathbf{X} \xrightarrow{r} 0$$

$$* \xrightarrow{r} \mathbf{A}$$

Kinetic differential equations:

$$\frac{\mathrm{d[A]}}{\mathrm{dt}} = \frac{\mathrm{d}a}{\mathrm{dt}} = r\,(a_0 - a) - (k_1 + k_3 x^2)\,a + (k_2 + k_4 x^2)\,x$$

$$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathbf{X}$$

$$\frac{\mathrm{d[X]}}{\mathrm{dt}} = \frac{\mathrm{d}x}{\mathrm{dt}} = -\,r\,x + (k_1 + k_3 x^2)\,a - (k_2 + k_4 x^2)\,x$$

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Steady states:

$$\bar{x}^3 (k_3 + k_4) - \bar{x}^2 k_3 a_0 + \bar{x}(k_1 + k_2 + r) - k_1 a_0 = 0$$

$$\mathbf{A} \xrightarrow{r} 0$$

$$k_1 = k_2 = \alpha,\ k_3 = k_4 = 1\text{:}\quad 2\bar{x}^3 - \bar{x}^2 a_0 + \bar{x}(r + 2\alpha) - \alpha a_0 = 0$$

Polynomial discriminant of the cubic equation:

$$\mathbf{X} \xrightarrow{r} 0$$

$$216\,\mathrm{D} = r^3 + r^2 \left(6\alpha - \frac{{a_0}^2}{8}\right) + r\,(12\alpha^2 - 5\alpha\,{a_0}^2) + 8\alpha^3 + 4\alpha^2 {a_0}^2 + \frac{\alpha\,{a_0}^4}{2} = 0$$

$\ast \xrightarrow{r} \mathbf{A}$

Kinetic differential equations:

$$\frac{\mathrm{d[A]}}{\mathrm{dt}} = \frac{\mathrm{d}a}{\mathrm{dt}} = r\,(a_0 - a) - (k_1 + k_3 x^2)\,a + (k_2 + k_4 x^2)\,x$$

$\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathbf{X}$

$$\frac{\mathrm{d[X]}}{\mathrm{dt}} = \frac{\mathrm{d}x}{\mathrm{dt}} = -\,r\,x + (k_1 + k_3 x^2)\,a - (k_2 + k_4 x^2)\,x$$

$\mathbf{A} + 2\,\mathbf{X} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} 3\mathbf{X}$

Steady states:

$$\bar{x}^3 (k_3 + k_4) - \bar{x}^2 k_3 a_0 + \bar{x}(k_1 + k_2 + r) - k_1 a_0 = 0$$

$\mathbf{A} \xrightarrow{r} 0$

$$k_1 = k_2 = \alpha,\ k_3 = k_4 = 1\text{:}\quad 2\bar{x}^3 - \bar{x}^2 a_0 + \bar{x}(r + 2\alpha) - \alpha a_0 = 0$$

Polynomial discriminant of the cubic equation:

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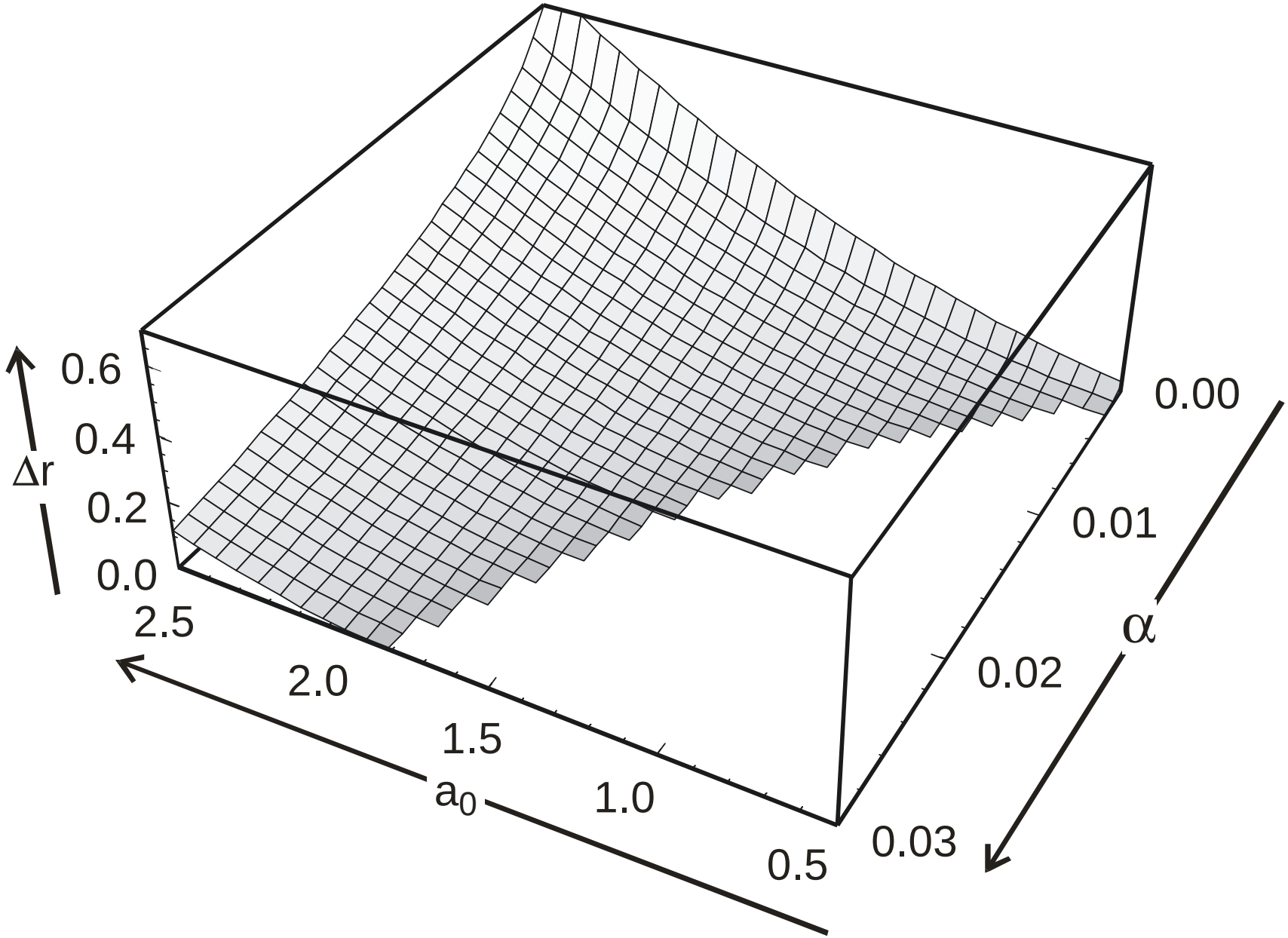
D < 0: 3 roots r_1, r_2, and r_3, 2 are positive $\Rightarrow$ $\Delta\mathbf{r} = r_1 - r_2$



Range of hysteresis as a function of the parameters a_0 and α

$$\frac{dc_i}{dt} = F_i(c_1, c_2, \cdots, c_n); \quad i = 1,2,\cdots,n \qquad \text{chemical reaction}$$

$$\frac{\partial c_i}{\partial t} = D_i \Delta c_i \qquad \text{diffusion}$$

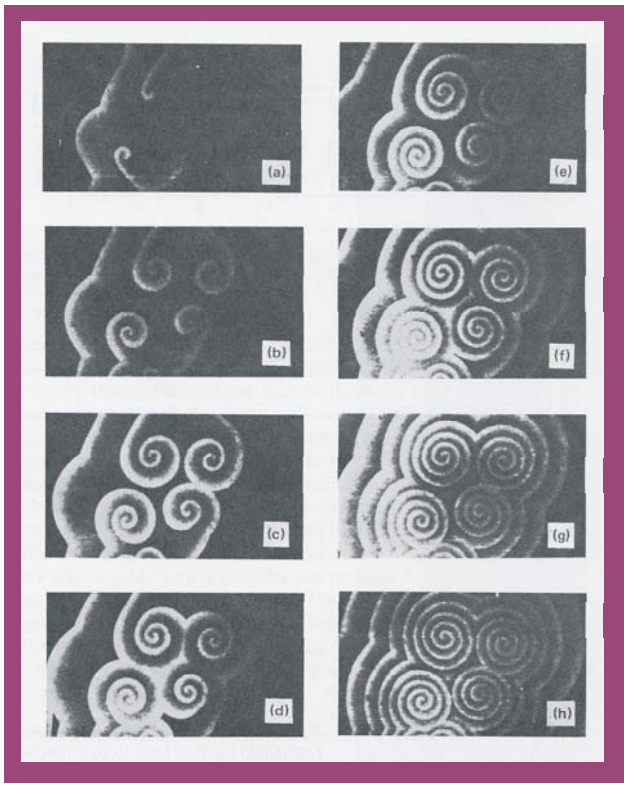
$$\Delta c_i = \left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right)$$

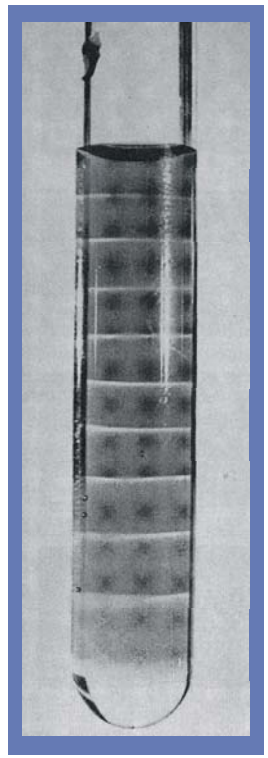
$$\frac{\partial c_i}{\partial t} = D_i \Delta c_i + F_i(c_1, c_2, \cdots, c_n); \quad i = 1,2,\cdots,n \qquad \text{reaction} - \text{diffusion}$$

Autocatalytic third order reactions

Direct, $A + 2X \rightarrow 3X$, or hidden in the reaction mechanism (Belousow-Zhabotinskii reaction).

- Multiple steady states
- Oscillations in homogeneous solution
- Deterministic chaos
- Turing patterns
- Spatiotemporal patterns (spirals)
  - Deterministic chaos in space and time





Pattern formation in autocatalytic third order reactions

G.Nicolis, I.Prigogine. *Self-Organization in Nonequilibrium Systems. From Dissipative Structures to Order through Fluctuations*. John Wiley, New York 1977

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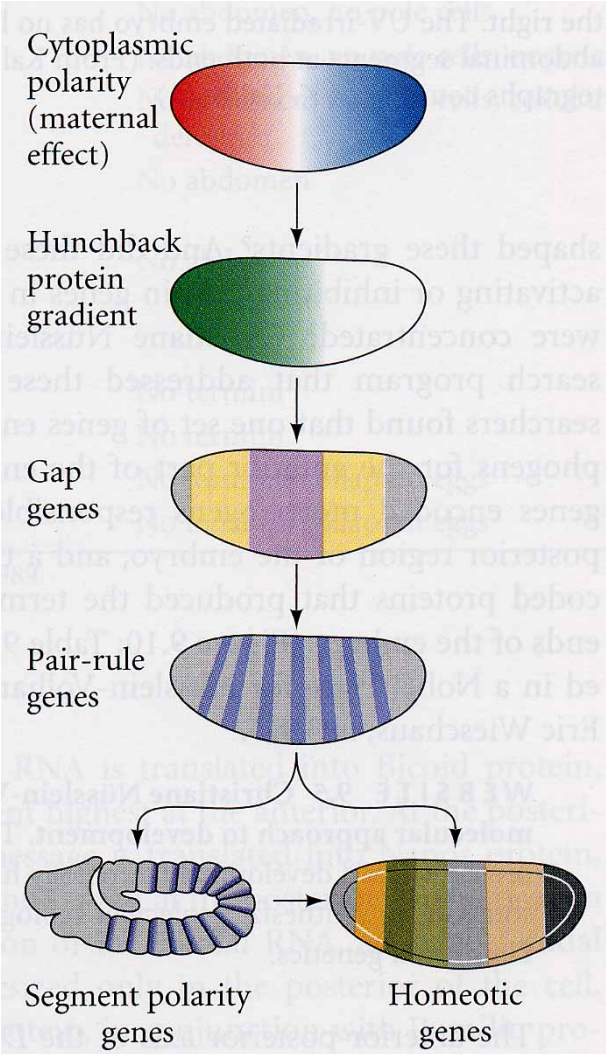
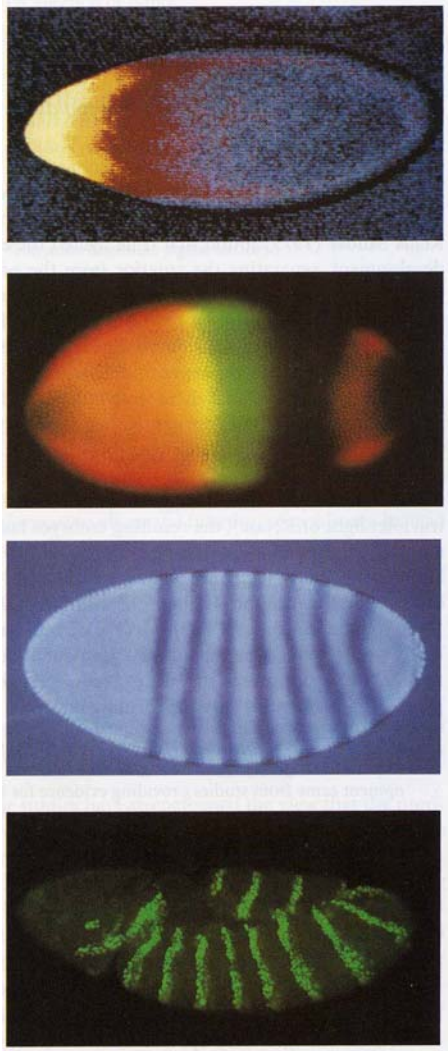
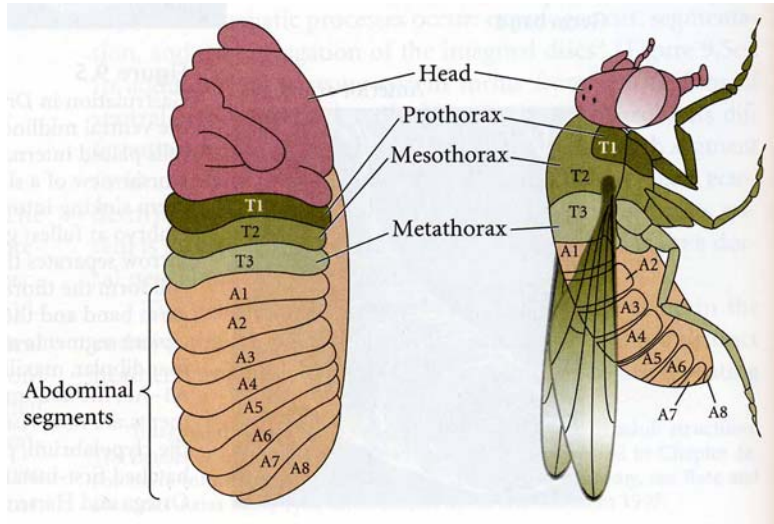
Gierer – Meinhardt model

$$\frac{\partial a}{\partial t} = D_a \Delta a + \frac{a^2}{(1+k a^2)\, h} - \mu\, a + \rho_a$$

$$\frac{\partial h}{\partial t} = D_h \Delta h + \rho a^2 - \nu\, h + \rho_h\,; \quad D_h > D_a$$







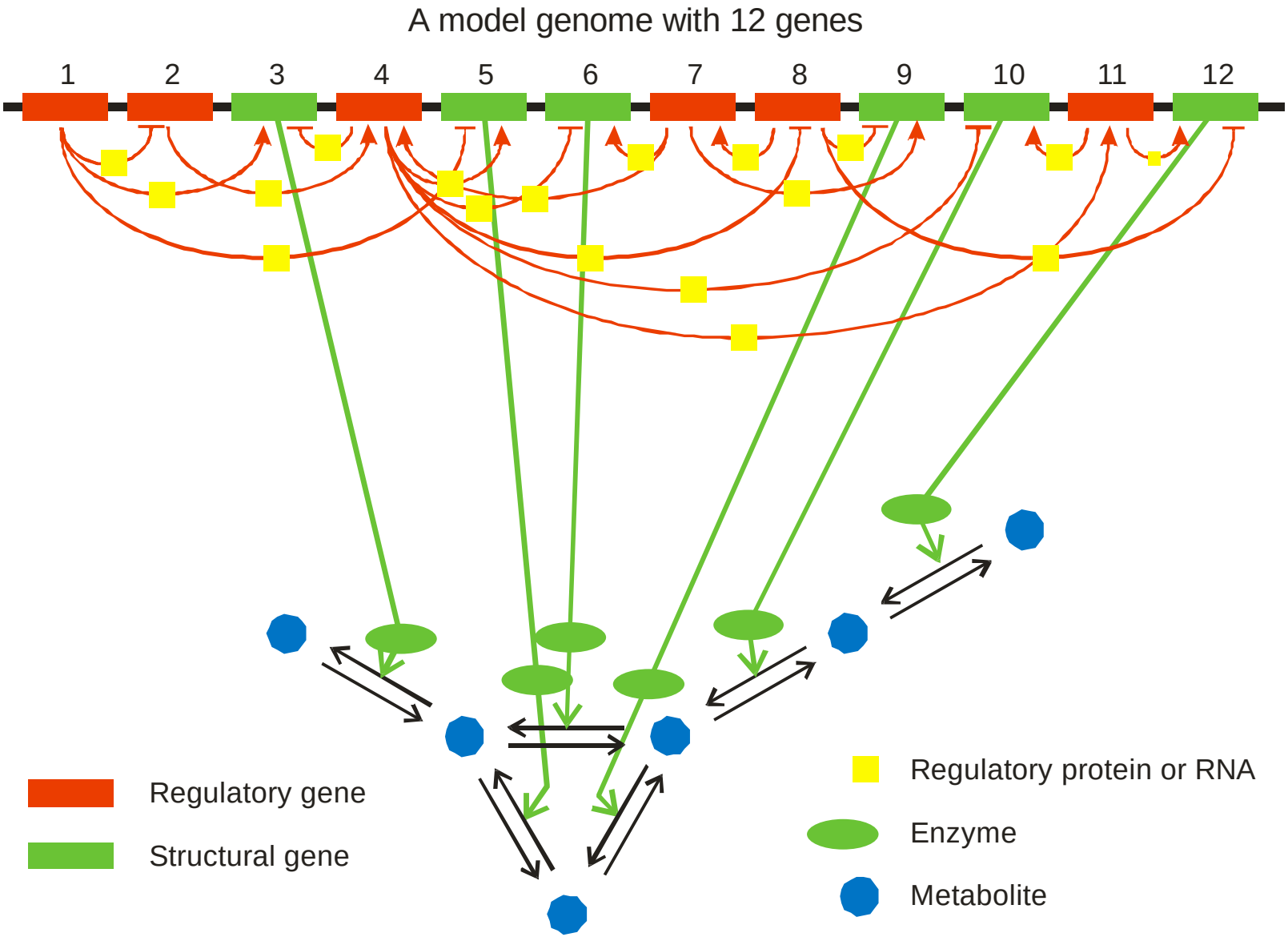
Cascades, A ⇒ B ⇒ C ⇒ ... , and networks of genetic control

Turing pattern resulting from reaction-diffusion equation ?

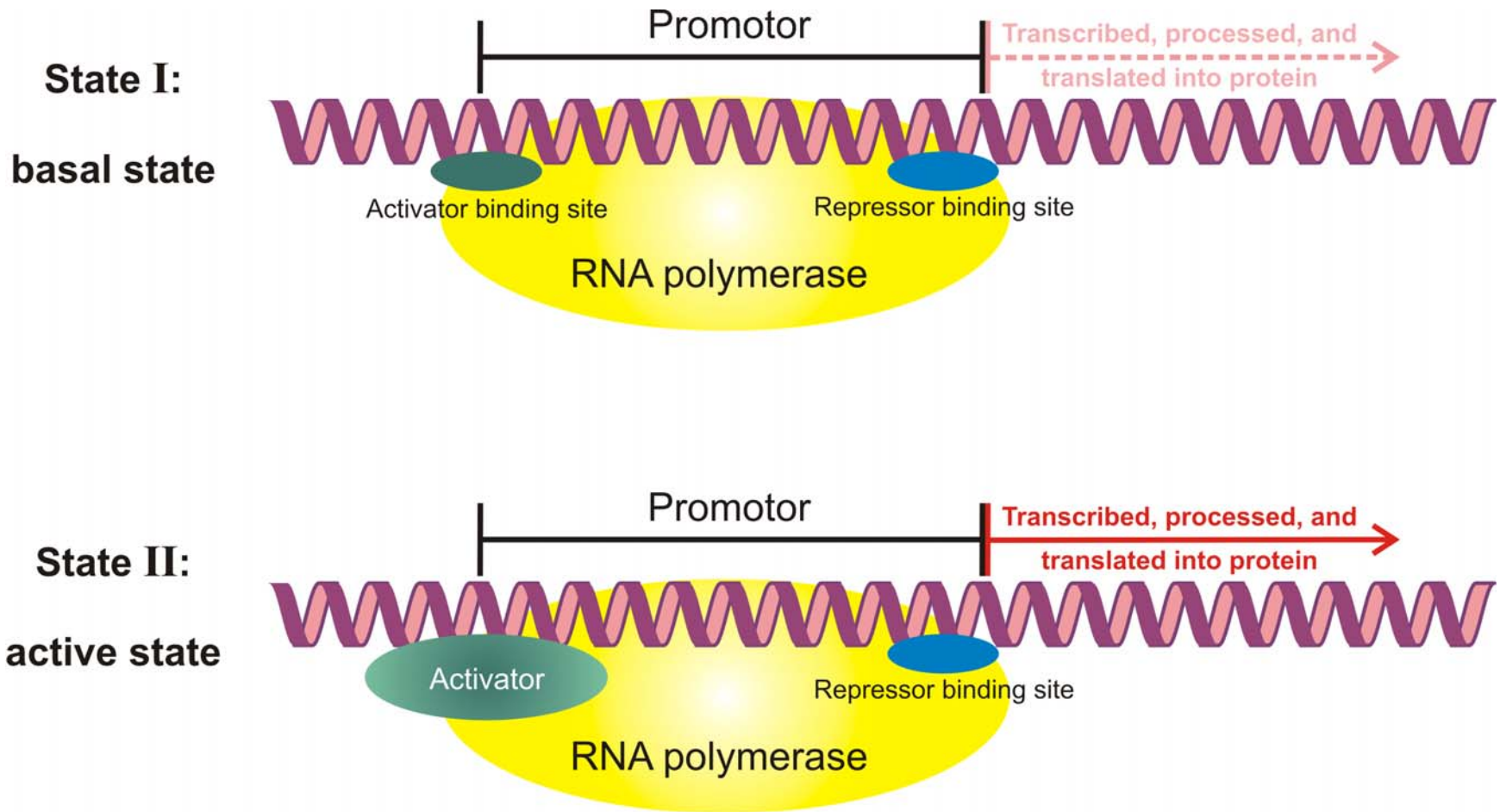
Intercelluar communication creating positional information

Development of the fruit fly *drosophila melanogaster*: Genetics, experiment, and imago

1. Equilibrium structures and dissipative patterns
2. Spatio-temporal patterns in chemical reactions
3. Patterns in development
4. **Genetic and metabolic networks**
5. Patterns in neurobiology



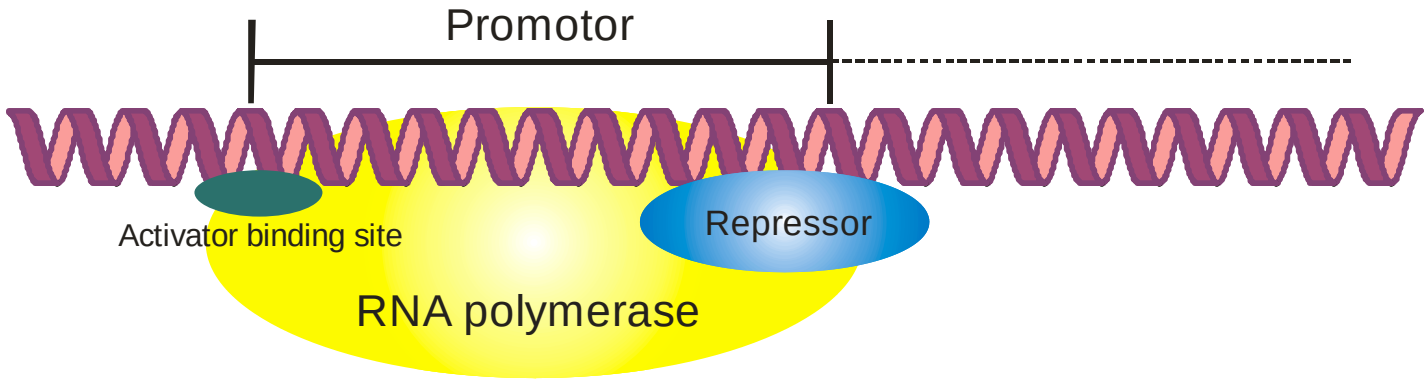
Sketch of a genetic and metabolic network



Active states of gene regulation

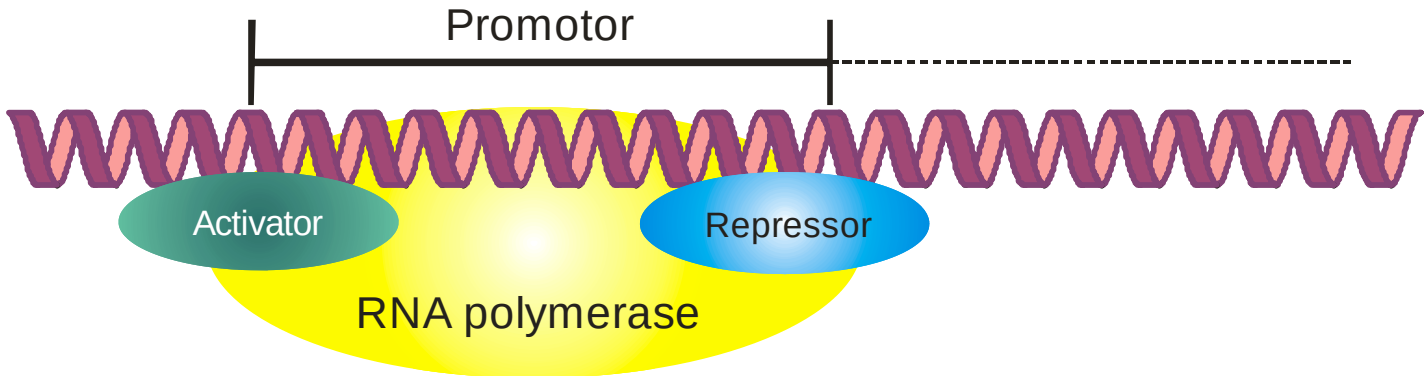
State III:

inactive state

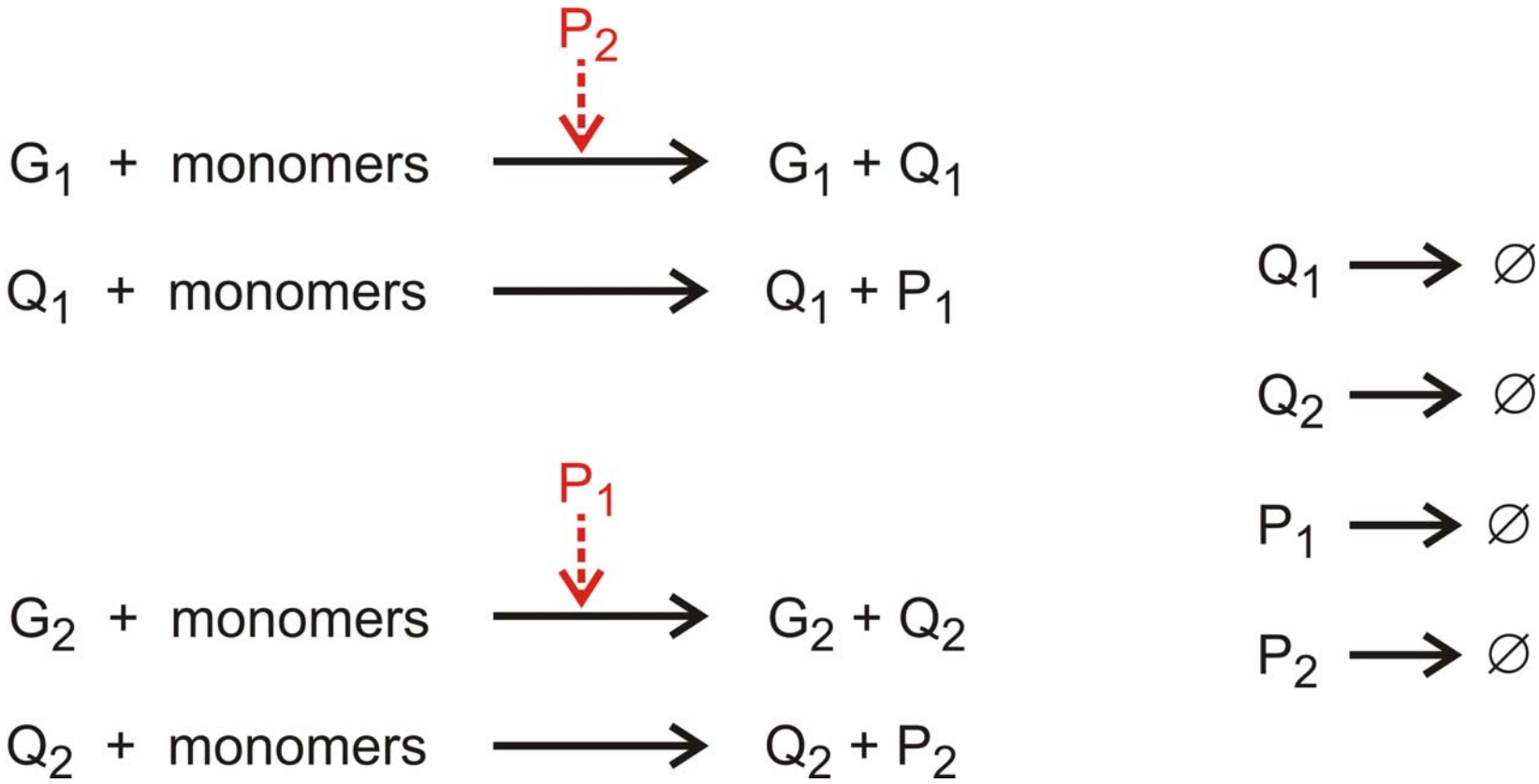


State III:

inactive state



Inactive states of gene regulation

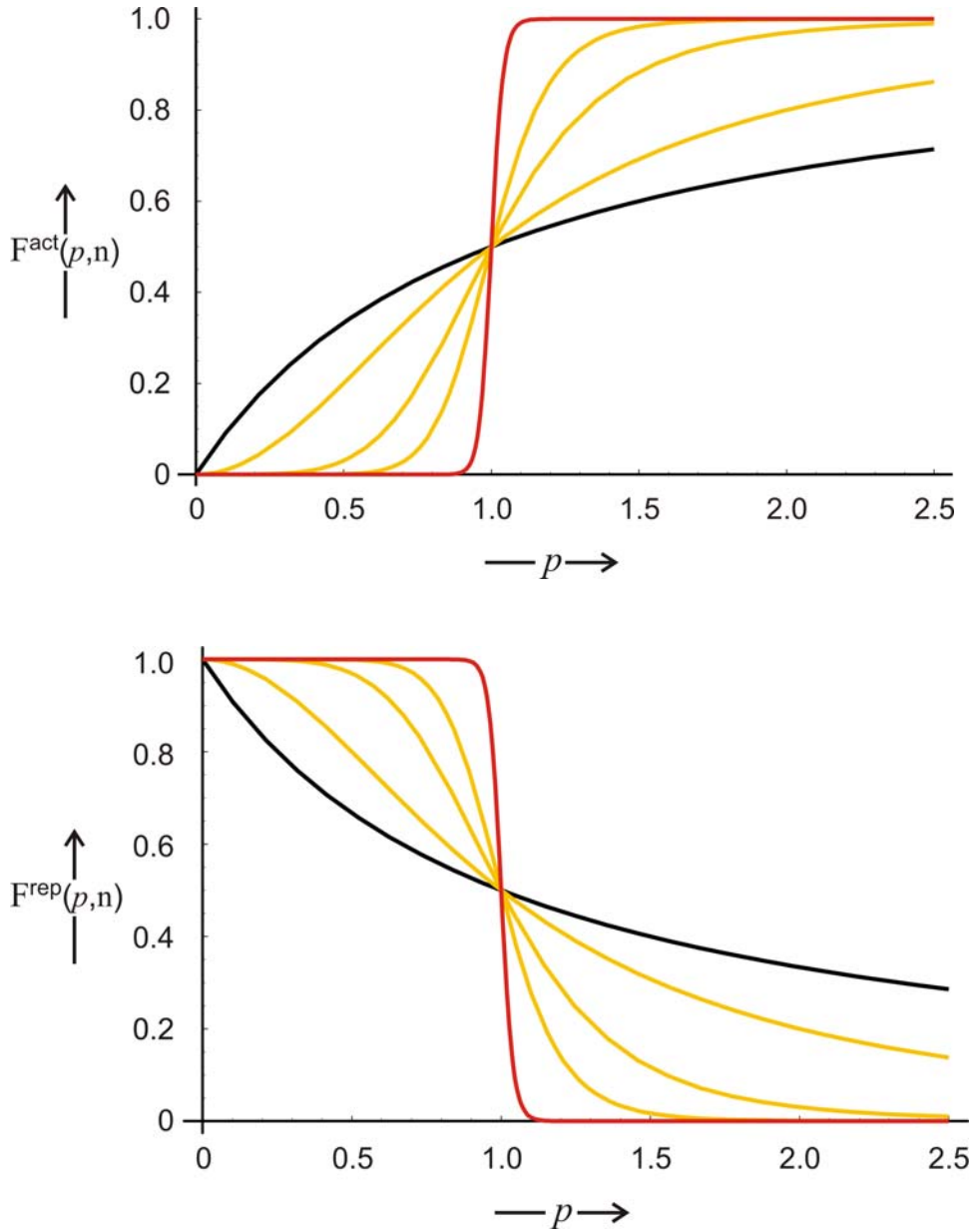


Cross-regulation of two genes

$$\text{Activation}: \quad F_i(p_j) = \frac{p_j^{\mathrm{n}}}{K + p_j^{\mathrm{n}}}$$

$$\text{Repression}: \quad F_i(p_j) = \frac{K}{K + p_j^{\mathrm{n}}}$$

$$i, j = 1,2$$



Gene regulatory binding functions

$[\mathrm{G}_1]=[\mathrm{G}_2]=g_0=\text{const.}$

$[\mathrm{Q}_1]=q_1,[\mathrm{Q}_2]=q_2,$

$[\mathrm{P}_1]=p_1,[\mathrm{P}_2]=p_2$

$$\text{Activation}: \quad F_i(p_j)=\frac{p_j^{\mathrm{n}}}{K+p_j^{\mathrm{n}}}$$

$$\text{Repression}: \quad F_i(p_j)=\frac{K}{K+p_j^{\mathrm{n}}}$$

$$i,j=1,2$$

$$\frac{dq_1}{dt}=k_1^{\mathrm{Q}}F_1(p_2)-d_1^{\mathrm{Q}}q_1$$

$$\frac{dq_2}{dt}=k_2^{\mathrm{Q}}F_2(p_1)-d_2^{\mathrm{Q}}q_2$$

$$\frac{dp_1}{dt}=k_1^{\mathrm{P}}q_1-d_2^{\mathrm{P}}p_1$$

$$\frac{dp_2}{dt}=k_2^{\mathrm{P}}q_2-d_2^{\mathrm{P}}p_2$$

$$\text{Stationary points}: \quad \bar{p}_1-\vartheta_1F_1(\vartheta_2F_2(\bar{p}_1))=0,\ \bar{p}_2=\vartheta_2F_2(\bar{p}_1)$$

$$\vartheta_1=\frac{k_1^{\mathrm{Q}}k_1^{\mathrm{P}}}{d_1^{\mathrm{Q}}d_1^{\mathrm{P}}},\ \vartheta_2=\frac{k_2^{\mathrm{Q}}k_2^{\mathrm{P}}}{d_2^{\mathrm{Q}}d_2^{\mathrm{P}}}$$

Qualitative analysis of cross-regulation of two genes: **Stationary points**

$$\mathrm{A} = \left\{ a_{ij} = \frac{\partial \dot{x}_i}{\partial x_j} \right\} = \begin{pmatrix} Q_D & Q_K \\ P_D & P_K \end{pmatrix} = \begin{pmatrix} -d_1^Q & 0 & k_1^Q \frac{\partial F_1}{\partial p_1} & k_1^Q \frac{\partial F_1}{\partial p_2} \\ 0 & -d_2^Q & k_2^Q \frac{\partial F_2}{\partial p_1} & k_2^Q \frac{\partial F_2}{\partial p_2} \\ k_1^P & 0 & -d_1^P & 0 \\ 0 & k_2^P & 0 & -d_2^P \end{pmatrix}$$

$$Q_D \cdot P_K = P_K \cdot Q_D \quad \text{and hence} \quad \begin{vmatrix} Q_D & Q_K \\ P_K & P_D \end{vmatrix} = \left| Q_D \cdot P_D - Q_K \cdot P_K \right|$$

$$\Gamma(\bar{p}_1, \bar{p}_2) = -\begin{vmatrix} 0 & \frac{\partial F_1}{\partial p_2} \\ \frac{\partial F_2}{\partial p_1} & 0 \end{vmatrix} = \frac{\partial F_1}{\partial p_2} \cdot \frac{\partial F_2}{\partial p_1}$$

Qualitative analysis of cross-regulation of two genes: **Jacobian matrix**

$$(\varepsilon + d_1^{\mathrm{Q}})(\varepsilon + d_2^{\mathrm{Q}})(\varepsilon + d_1^{\mathrm{P}})(\varepsilon + d_2^{\mathrm{P}}) + D = 0$$

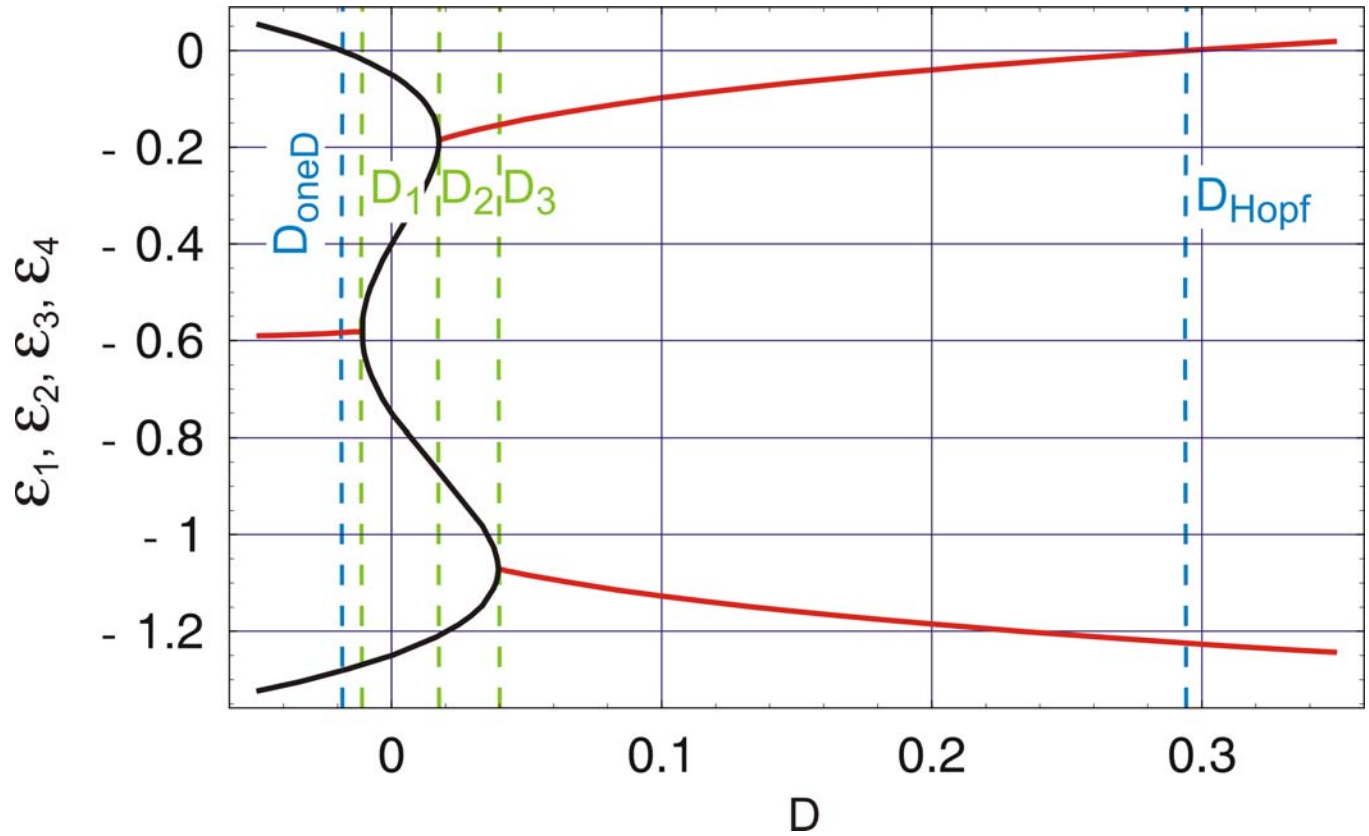
$$D = -k_1^{\mathrm{Q}} k_2^{\mathrm{Q}} k_1^{\mathrm{P}} k_2^{\mathrm{P}} \Gamma(\overline{p}_1, \overline{p}_2)$$

$$\Gamma(\overline{p}_1, \overline{p}_2) = -\begin{vmatrix} 0 & \dfrac{\partial F_1}{\partial p_2} \\ \dfrac{\partial F_2}{\partial p_1} & 0 \end{vmatrix} = \frac{\partial F_1}{\partial p_2} \cdot \frac{\partial F_2}{\partial p_1}$$

$$(\varepsilon + d_1^{\mathrm{Q}})(\varepsilon + d_2^{\mathrm{Q}})(\varepsilon + d_1^{\mathrm{P}})(\varepsilon + d_2^{\mathrm{P}}) + D = 0$$

Eigenvalues of the Jacobian of the cross-regulatory two gene system

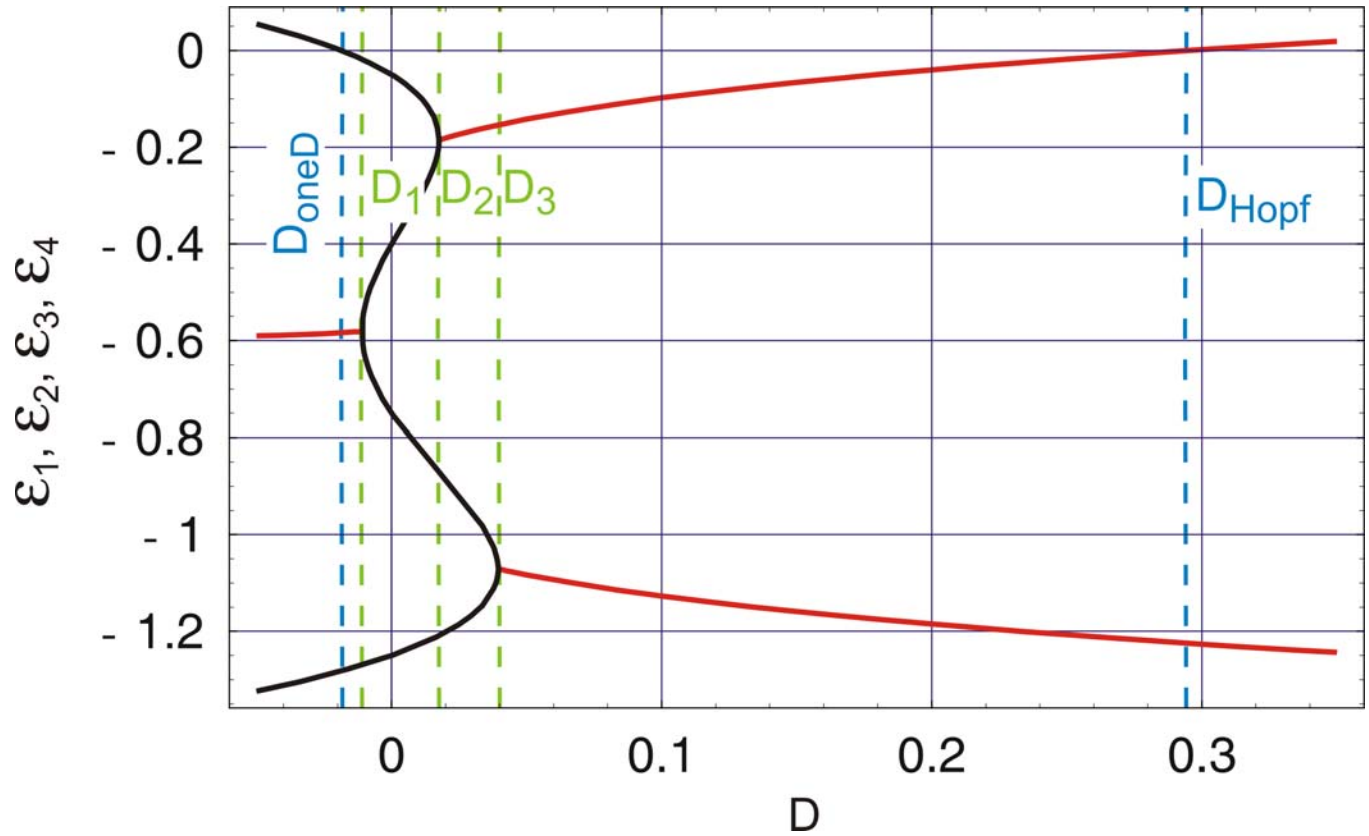
$$D = -k_1^{\mathrm{Q}} k_2^{\mathrm{Q}} k_1^{\mathrm{P}} k_2^{\mathrm{P}} \Gamma(\overline{p}_1, \overline{p}_2)$$



$$(\varepsilon + d_1^{\mathrm{Q}})(\varepsilon + d_2^{\mathrm{Q}})(\varepsilon + d_1^{\mathrm{P}})(\varepsilon + d_2^{\mathrm{P}}) + D = 0$$

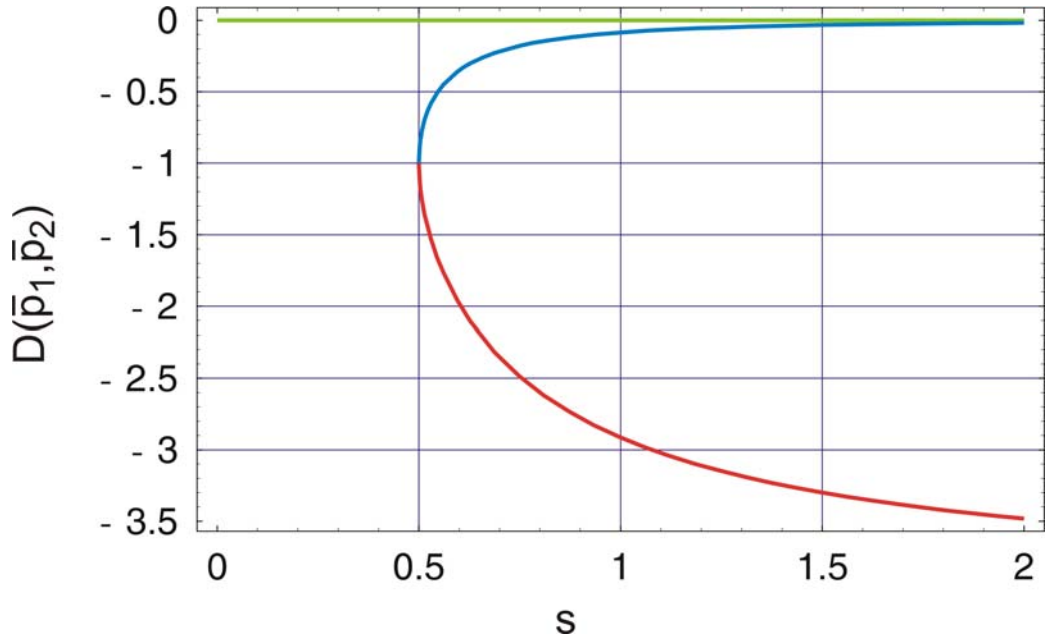
Eigenvalues of the Jacobian of the cross-regulatory two gene system

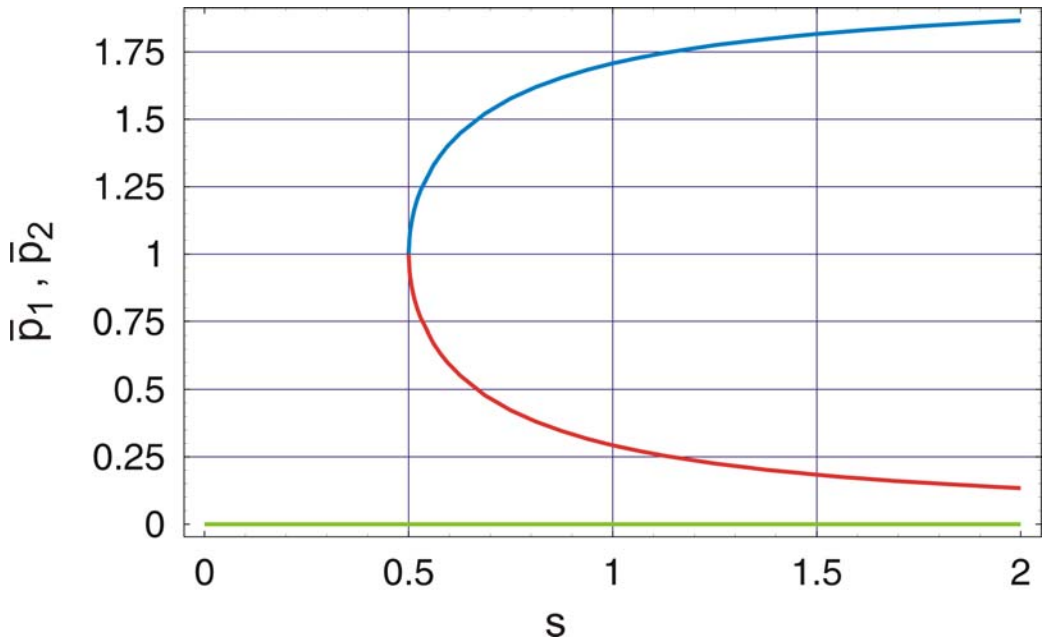
$$D = -k_1^{\mathrm{Q}} k_2^{\mathrm{Q}} k_1^{\mathrm{P}} k_2^{\mathrm{P}} \Gamma(\bar{p}_1, \bar{p}_2)$$



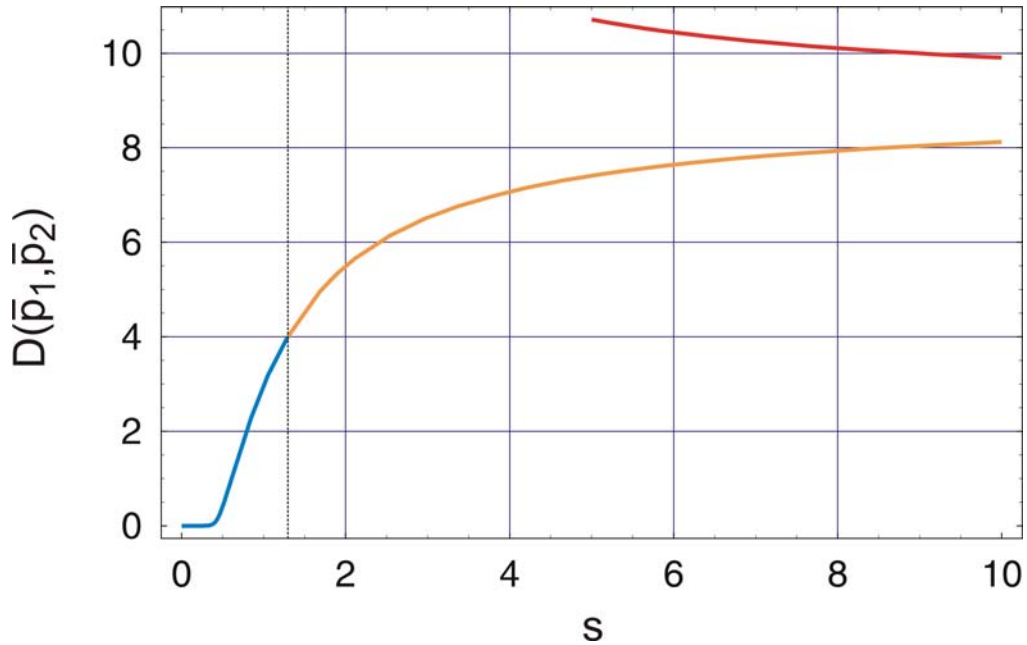
$$D_{\mathrm{OneD}} = -d_1^{\mathrm{Q}} d_2^{\mathrm{Q}} d_1^{\mathrm{P}} d_2^{\mathrm{P}}$$

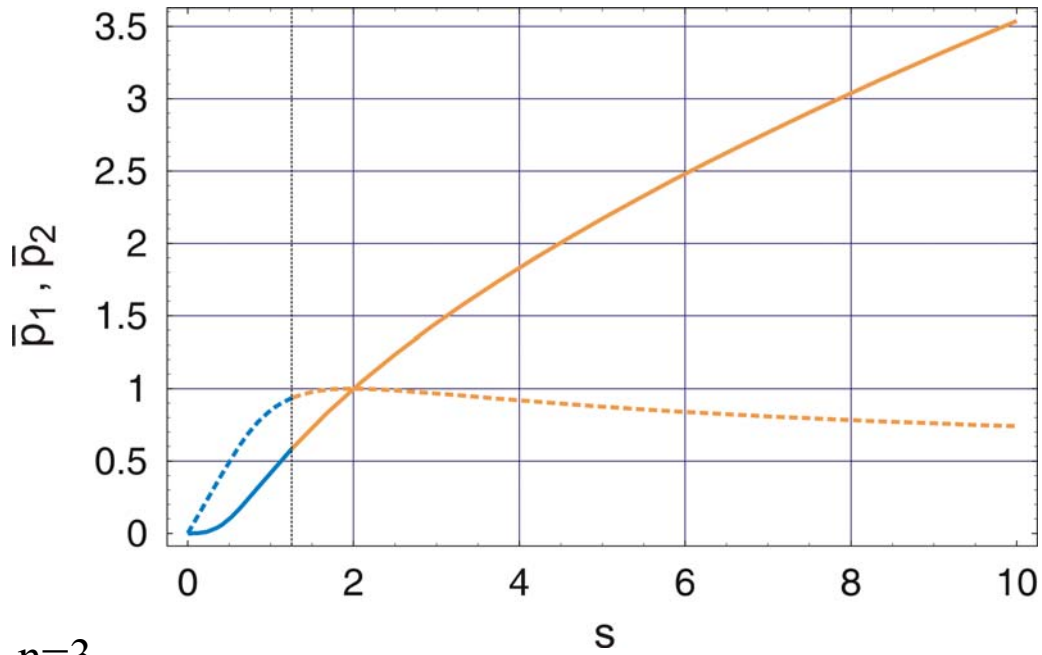
$$D_{\mathrm{Hopf}} = \frac{(d_1^{\mathrm{Q}}+d_2^{\mathrm{Q}})(d_1^{\mathrm{Q}}+d_1^{\mathrm{P}})(d_1^{\mathrm{Q}}+d_2^{\mathrm{P}})(d_2^{\mathrm{Q}}+d_1^{\mathrm{P}})(d_2^{\mathrm{Q}}+d_2^{\mathrm{P}})(d_1^{\mathrm{P}}+d_2^{\mathrm{P}})}{(d_1^{\mathrm{Q}}+d_2^{\mathrm{Q}}+d_1^{\mathrm{P}}+d_2^{\mathrm{P}})^2}$$



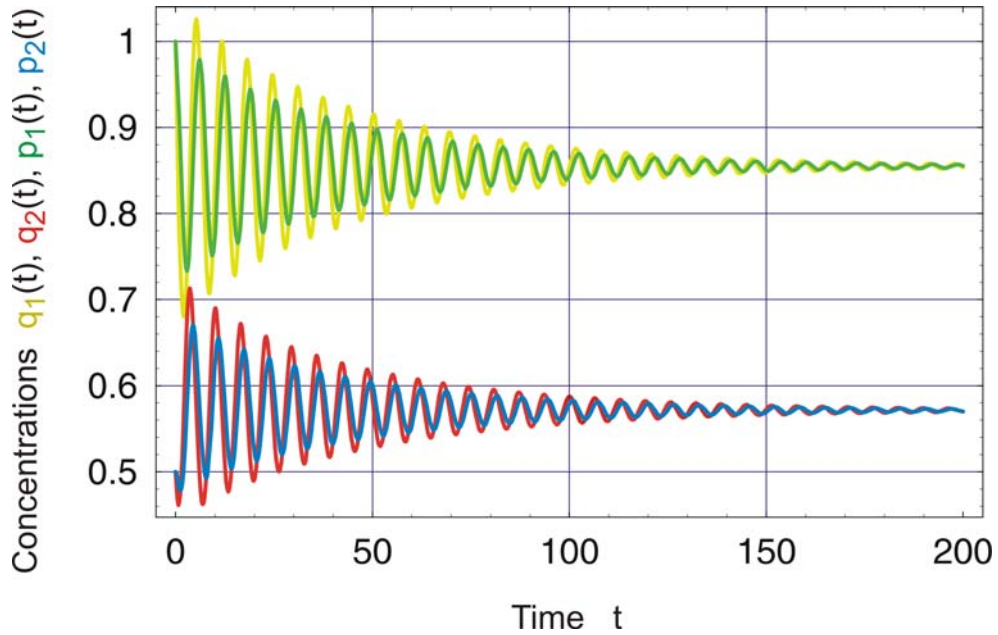


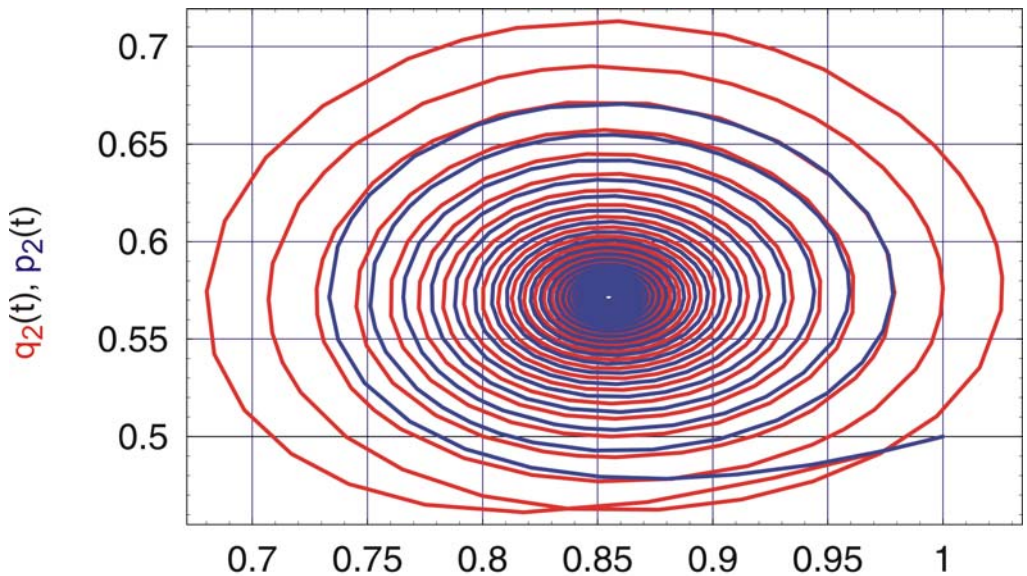
Regulatory dynamics at $D \leq 0$, act.-act., n=2



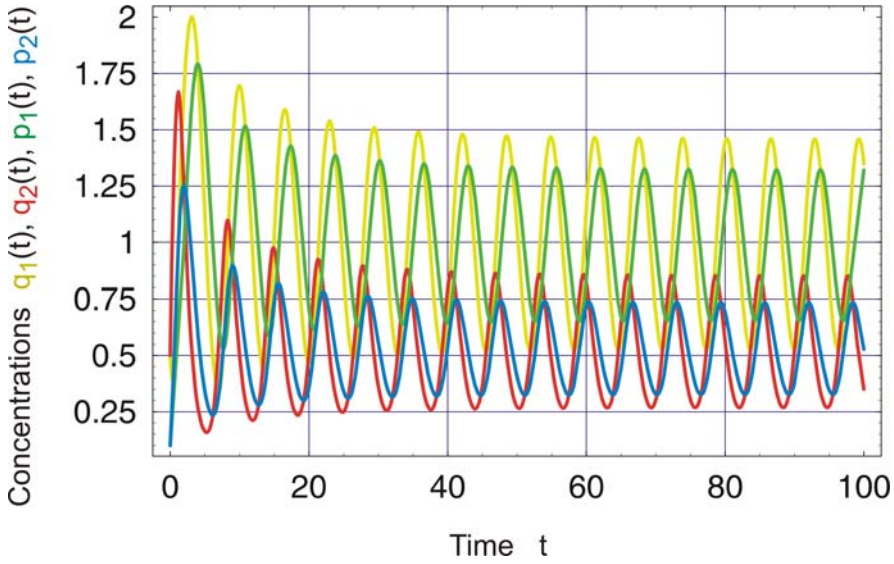


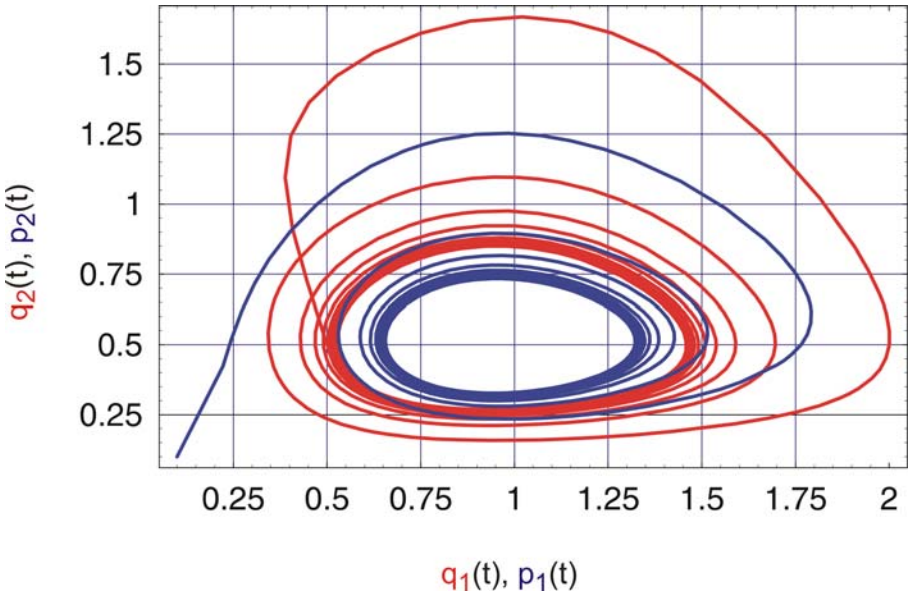
Regulatory dynamics at $D \geq 0$, act.-rep., n=3

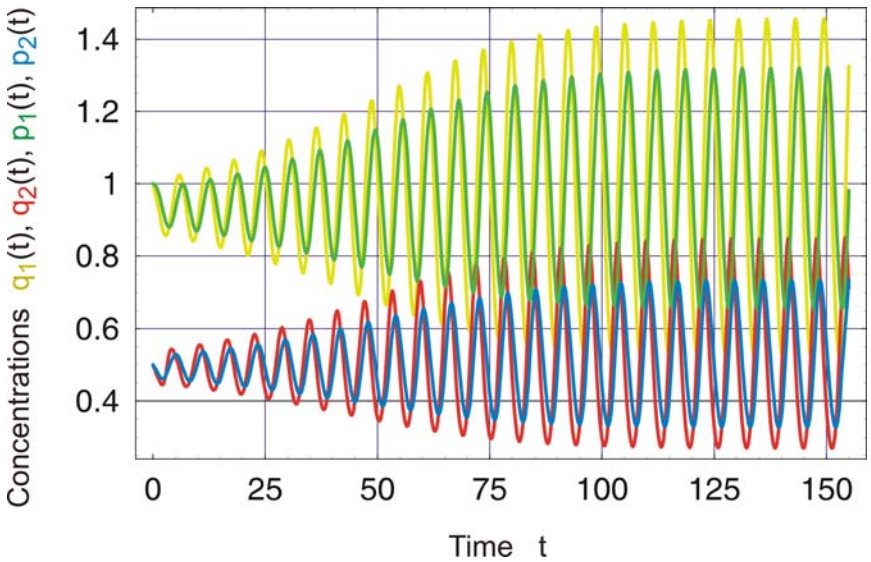


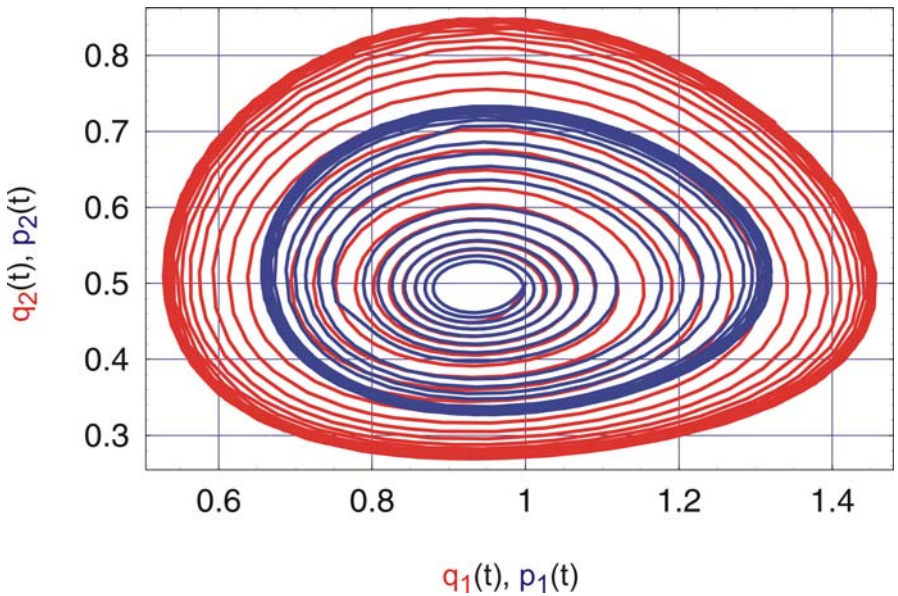


Regulatory dynamics at $D < D_{Hopf}$, act.-repr., n=3

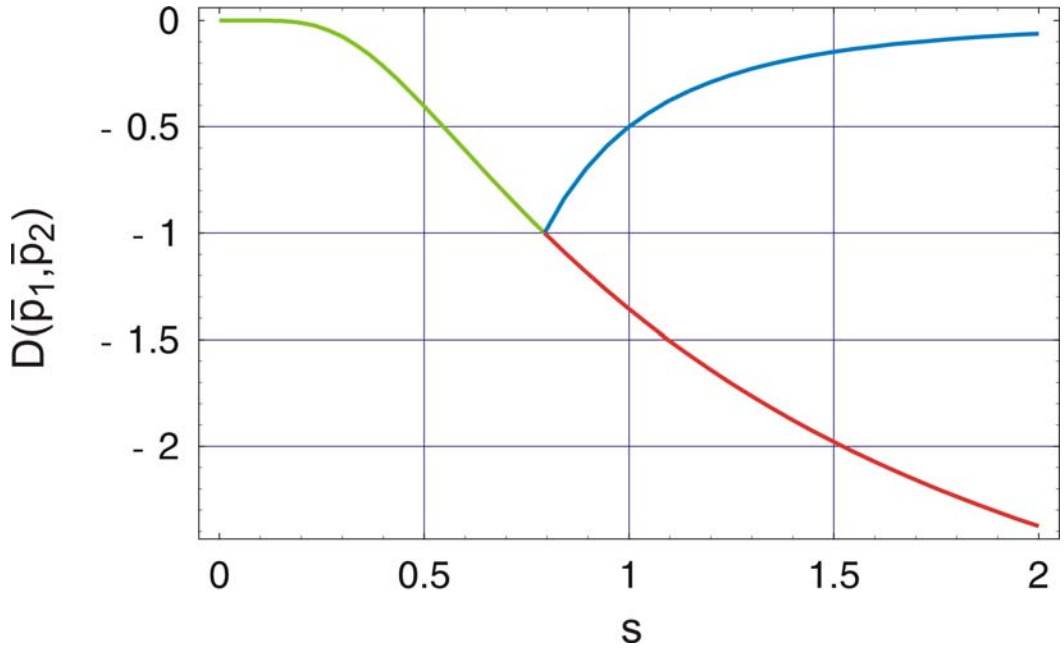


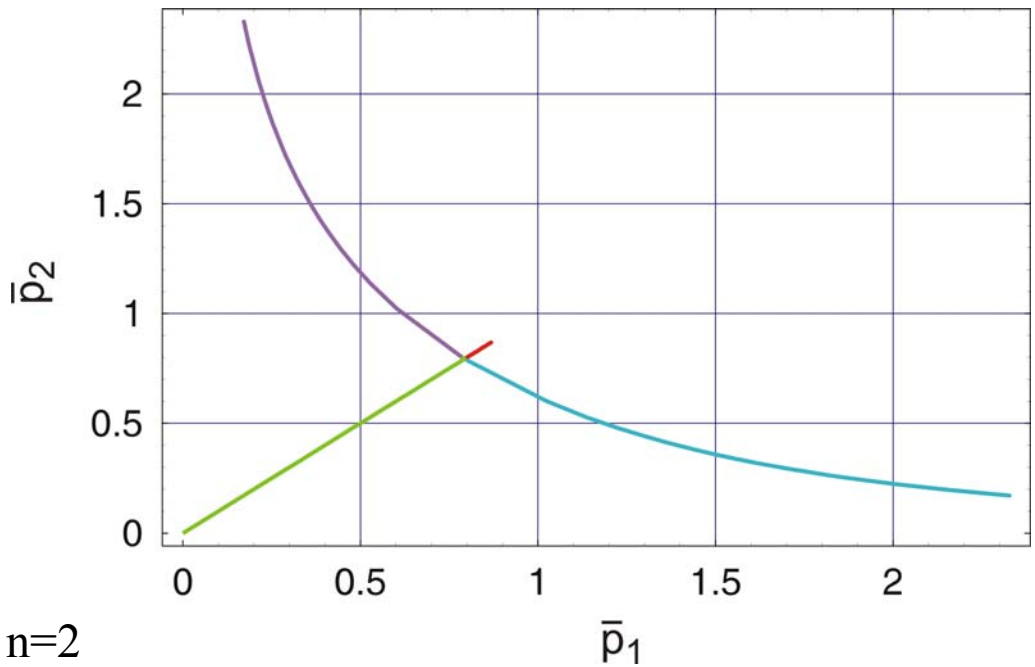






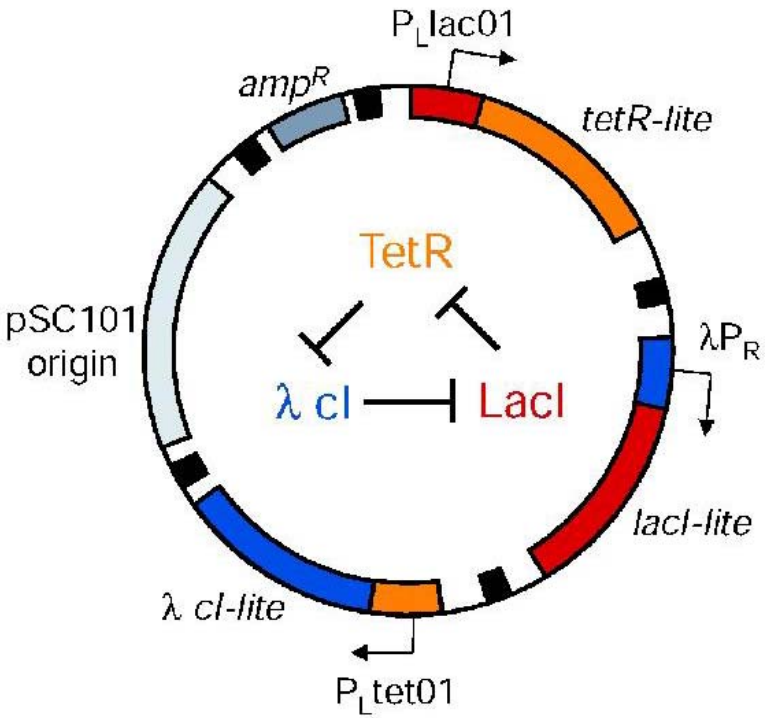
Regulatory dynamics at $D > D_{Hopf}$, act.-repr., n=3

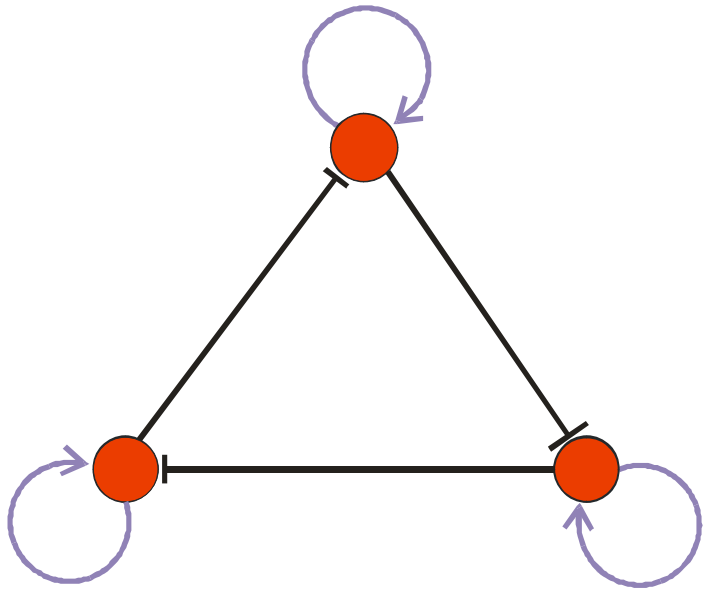




Regulatory dynamics at $D \leq 0$, rep.-rep., n=2

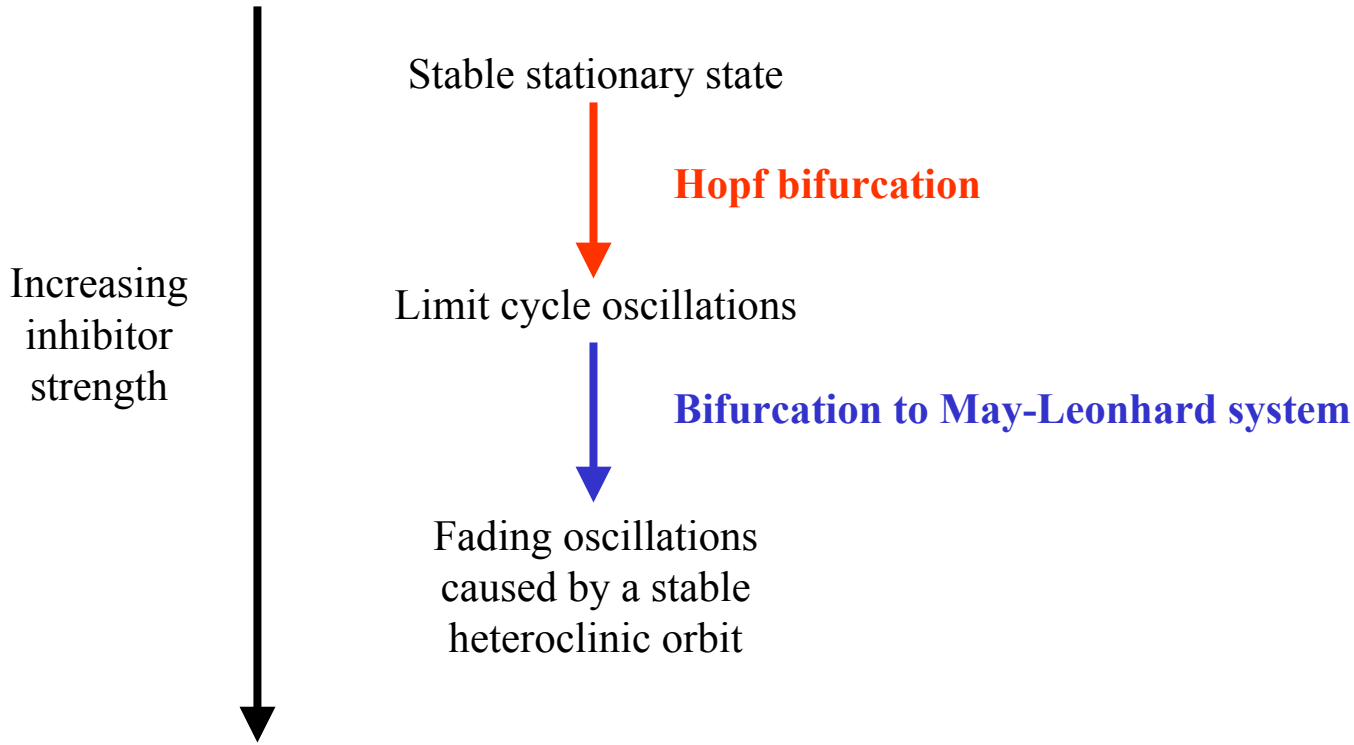
Hill coefficient: n	Act.-Act.	Act.-Rep.	Rep.-Rep.
1	S , E	S	S
2	E , B(E,P)	S	S , B(P_1,P_2)
3	E , B(E,P)	S , O	S , B(P_1,P_2)
4	E , B(E,P)	S , O	S , B(P_1,P_2)

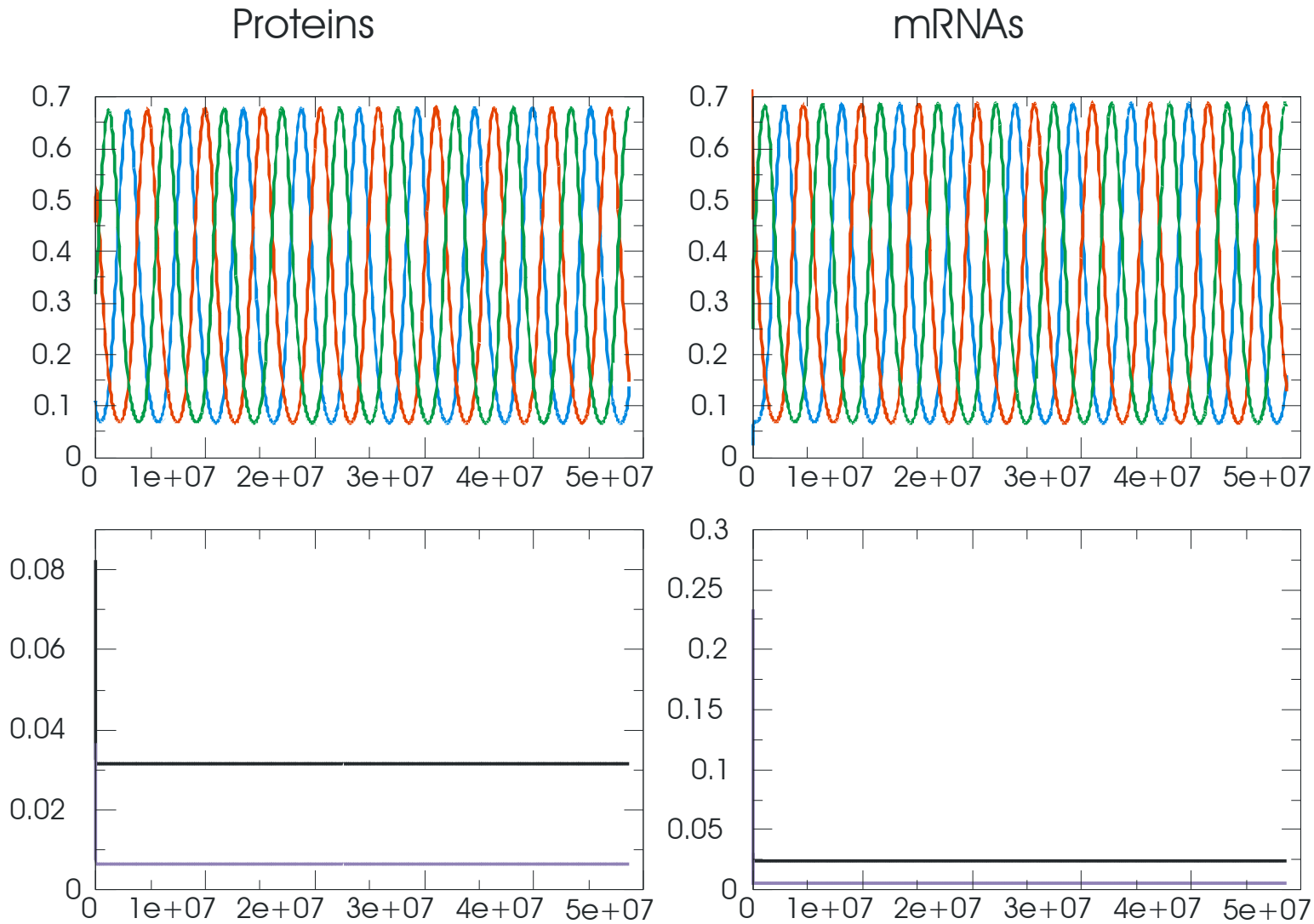




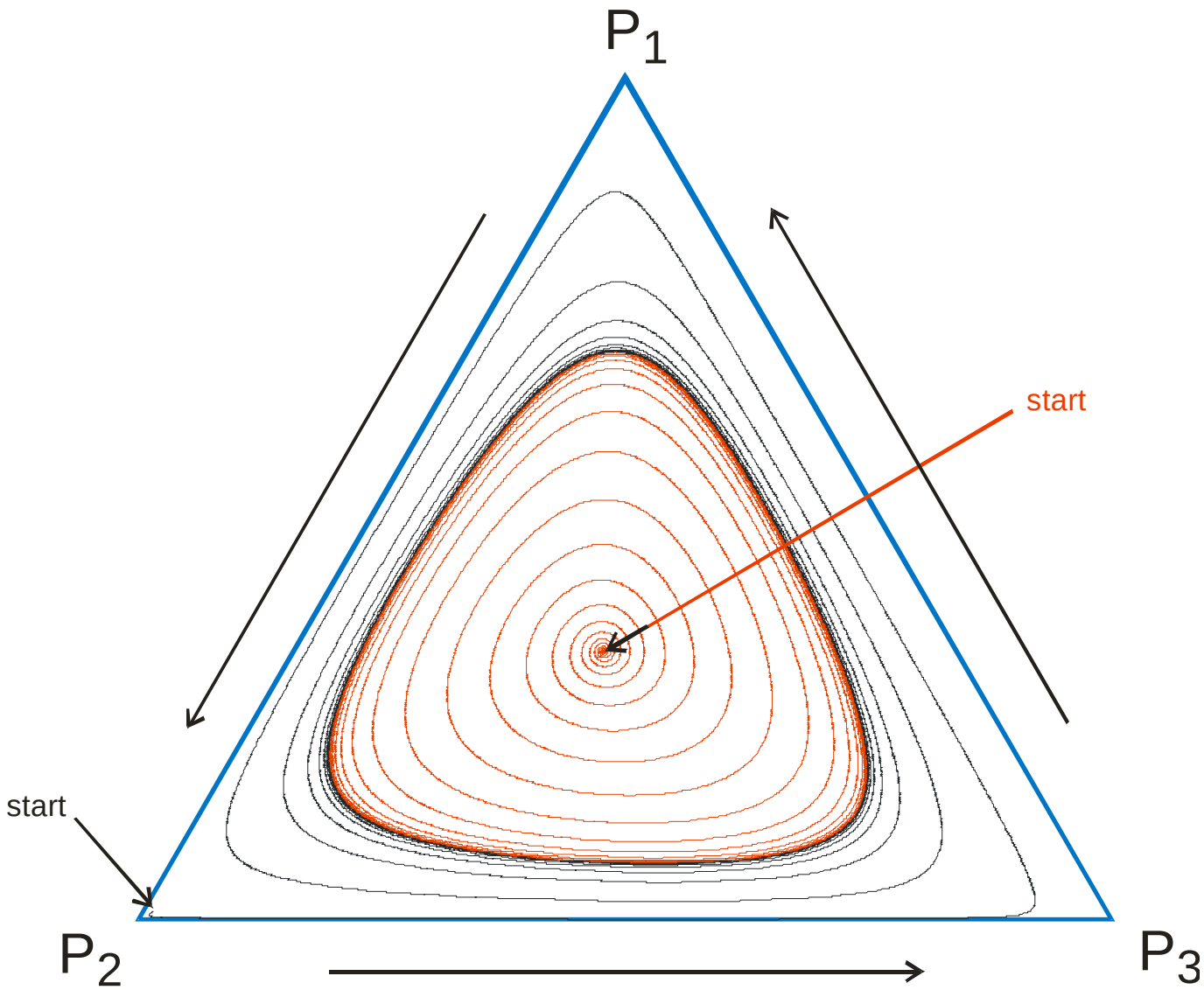
An example analyzed and simulated by MiniCellSim

The repressilator: M.B. Ellowitz, S. Leibler. A synthetic oscillatory network of transcriptional regulators. *Nature* **403**:335-338, 2002

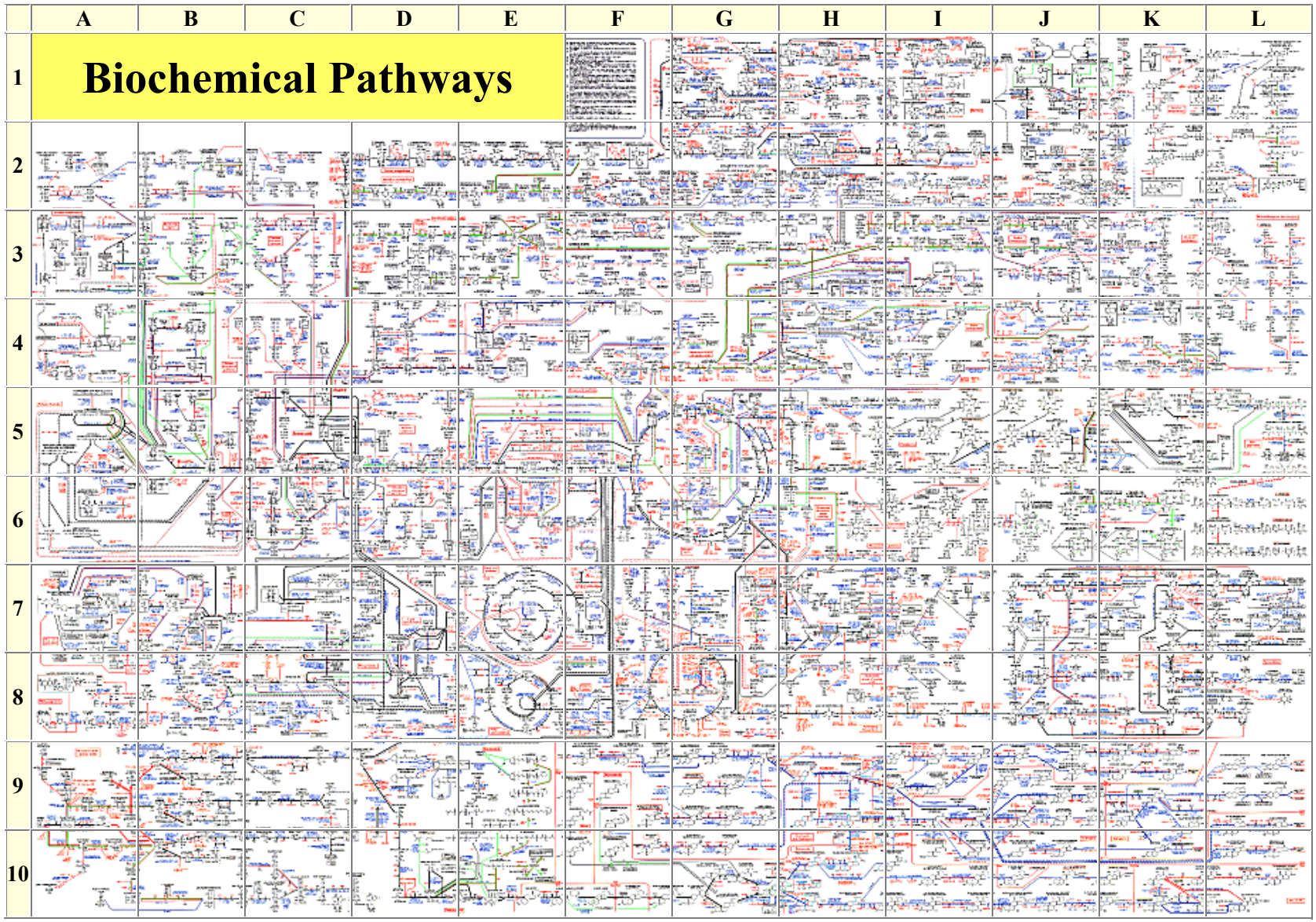

Increasing inhibitor strength
Stable stationary state
Hopf bifurcation
Limit cycle oscillations
Bifurcation to May-Leonhard system
Fading oscillations caused by a stable heteroclinic orbit



The repressilator limit cycle

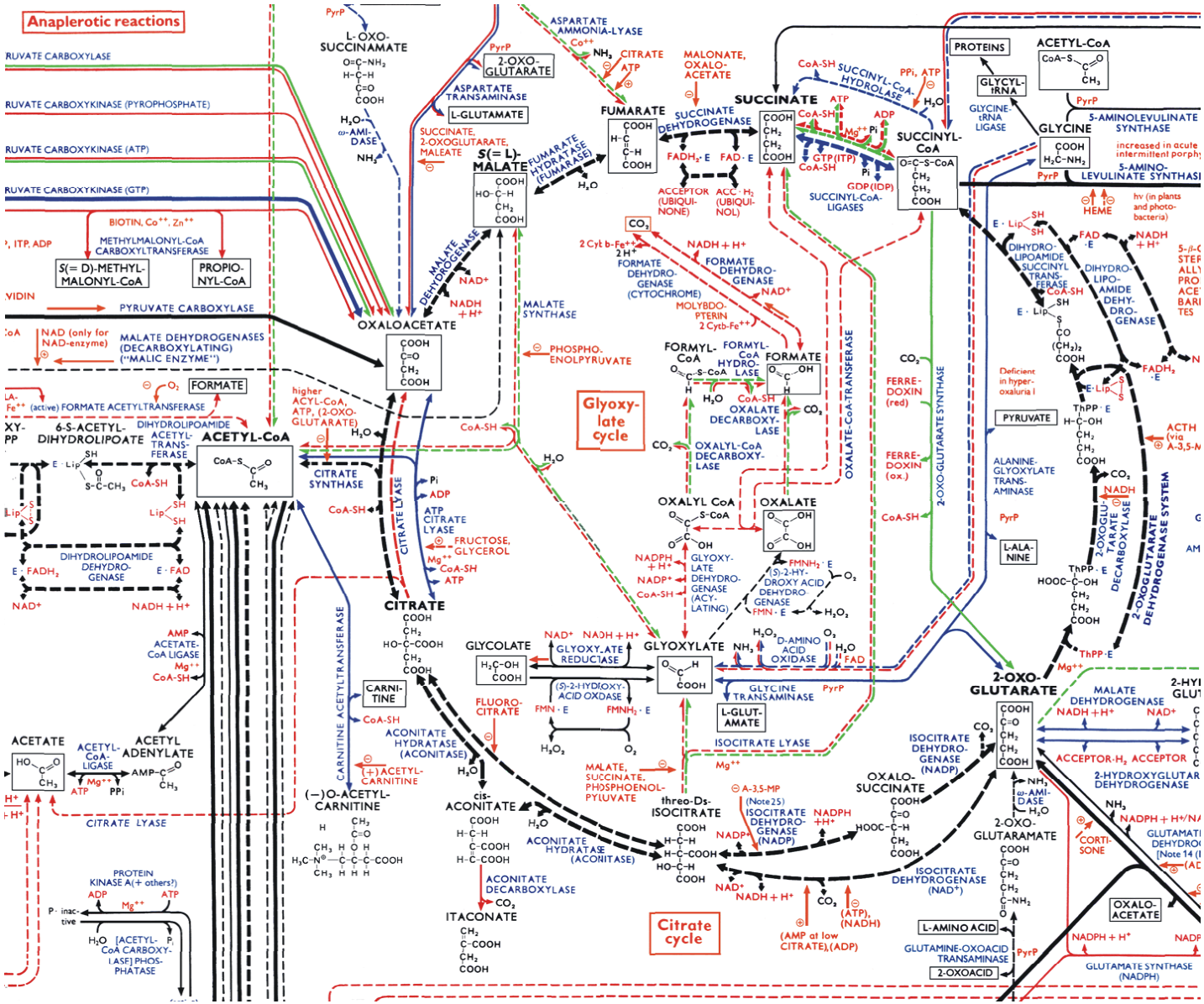


The repressilator limit cycle

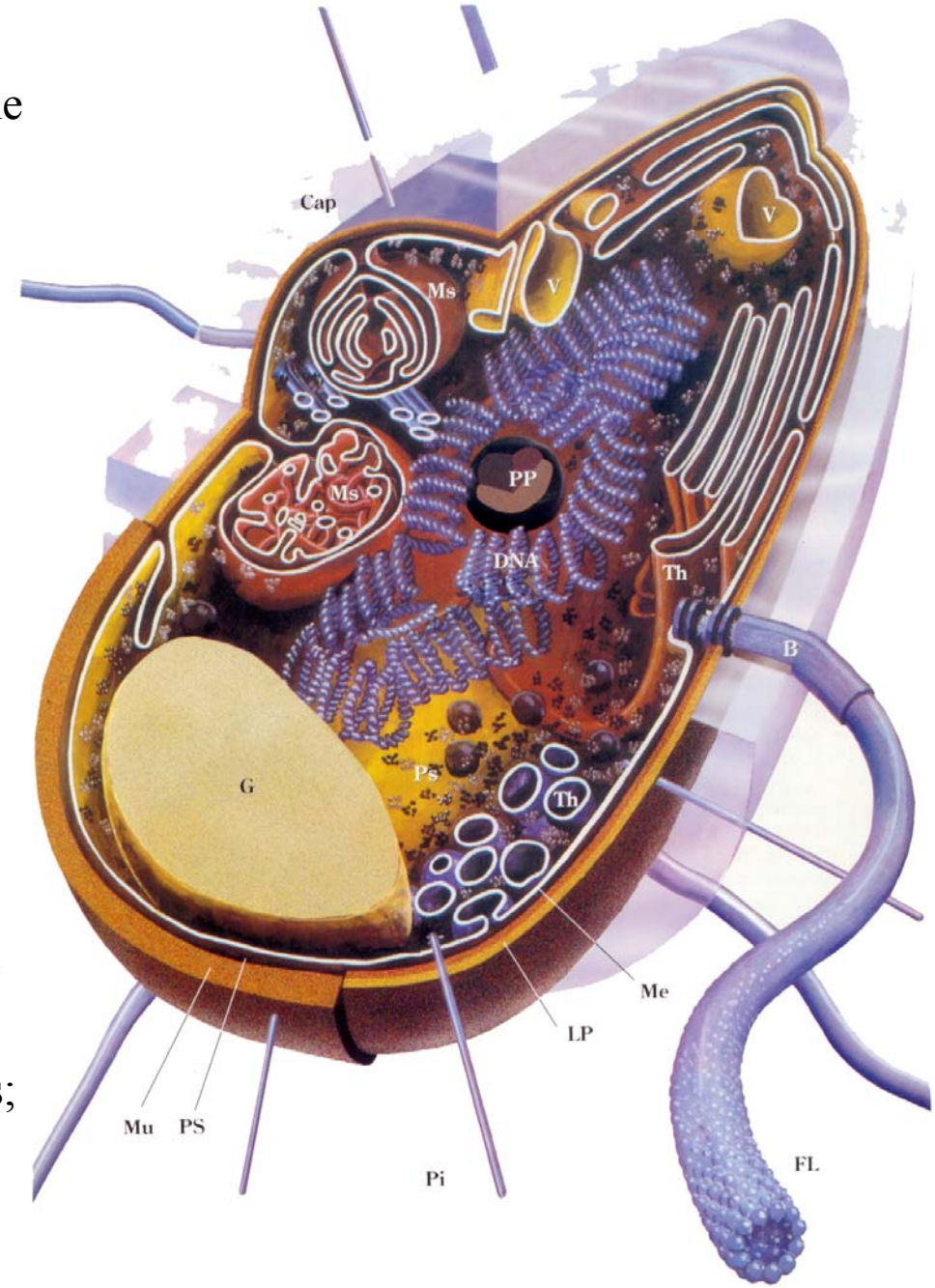


The reaction network of cellular metabolism published by Boehringer-Ingelheim.

The citric acid or Krebs cycle (enlarged from previous slide).



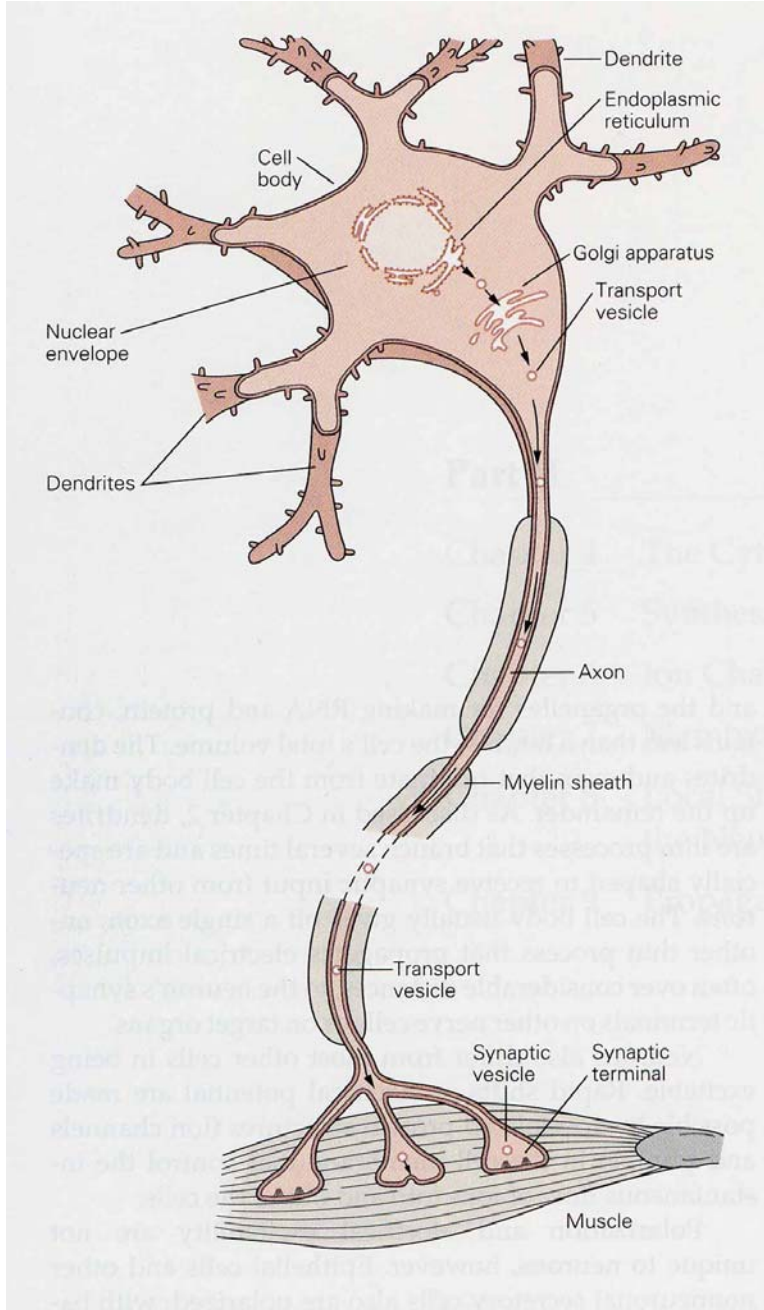
The **bacterial cell** as an example for the simplest form of autonomous life



The **human body**:

10^{14} cells = 10^{13} eukaryotic cells +
$\approx 9 \times 10^{13}$ bacterial (prokaryotic) cells;
$\approx$ 200 eukaryotic cell types

1. Equilibrium structures and dissipative patterns
2. Spatio-temporal patterns in chemical reactions
3. Patterns in development
4. Genetic and metabolic networks
5. **Patterns in neurobiology**



A single neuron signaling to a muscle fiber

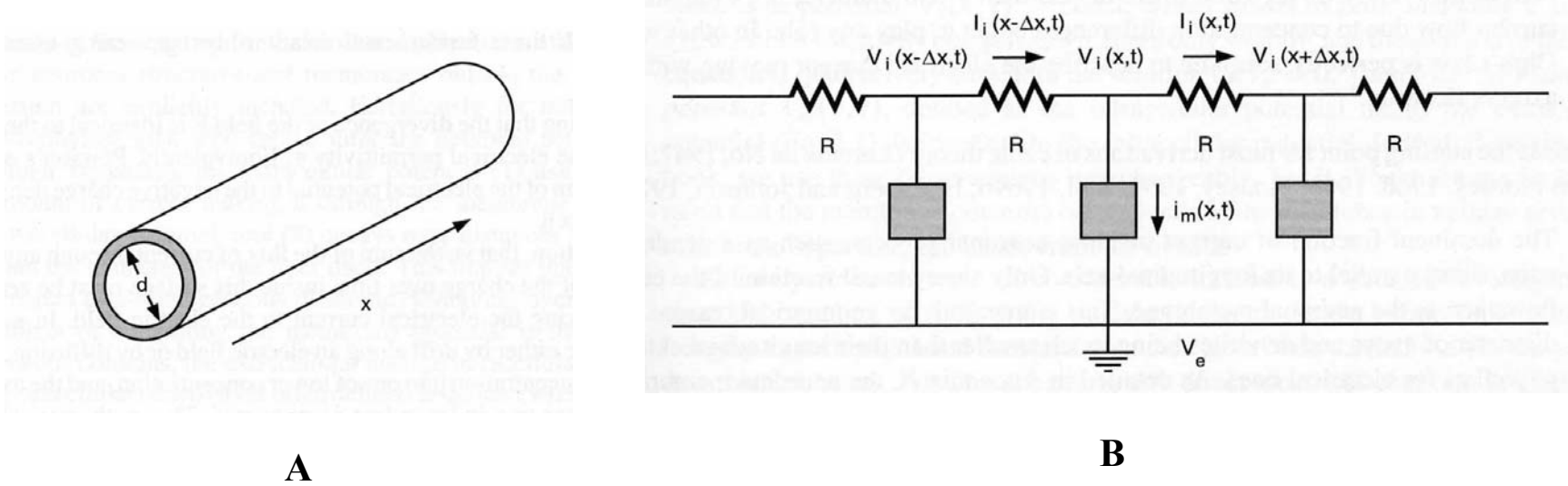


Fig. 2.2 ELECTRICAL STRUCTURE OF A CABLE **(A)** Idealized cylindrical axon or dendrite at the heart of one-dimensional cable theory. Almost all of the current inside the cylinder is longitudional due to geometrical (the radius is much smaller than the length of the cable) and electrical factors (the membrane covering the axon or dendrite possesses a very high resistivity compared to the intracellular cytoplasm). As a consequence, the radial and angular components of the current can be neglected, and the problem of determining the potential in these structures can be reduced from three spatial dimensions to a single one. On the basis of the bidomain approximation, gradients in the extracellular potentials are neglected and the cable problem is expressed in terms of the transmembrane potential $V_m(x,t) = V_i(x,t) - V_e$. **(B)** Equivalent electrical structure of an arbitrary neuronal process. The intracellular cytoplasm is modeled by the purely ohmic resistance R. This tacitly assumes that movement of carriers is exclusively due to drift along the voltage gradient and not to diffusion. Here and in the following the extracellular resistance is assumed to be negligible and V_e is set to zero. The current per unit length across the membrane, whether it is passive or contains voltage-dependent elements, is described by i_m and the system is characterized by the second-order differential equation, Eq. 2.5.

Christof Koch, Biophysics of Computation. Information Processing in single neurons.
Oxford University Press, New York 1999.

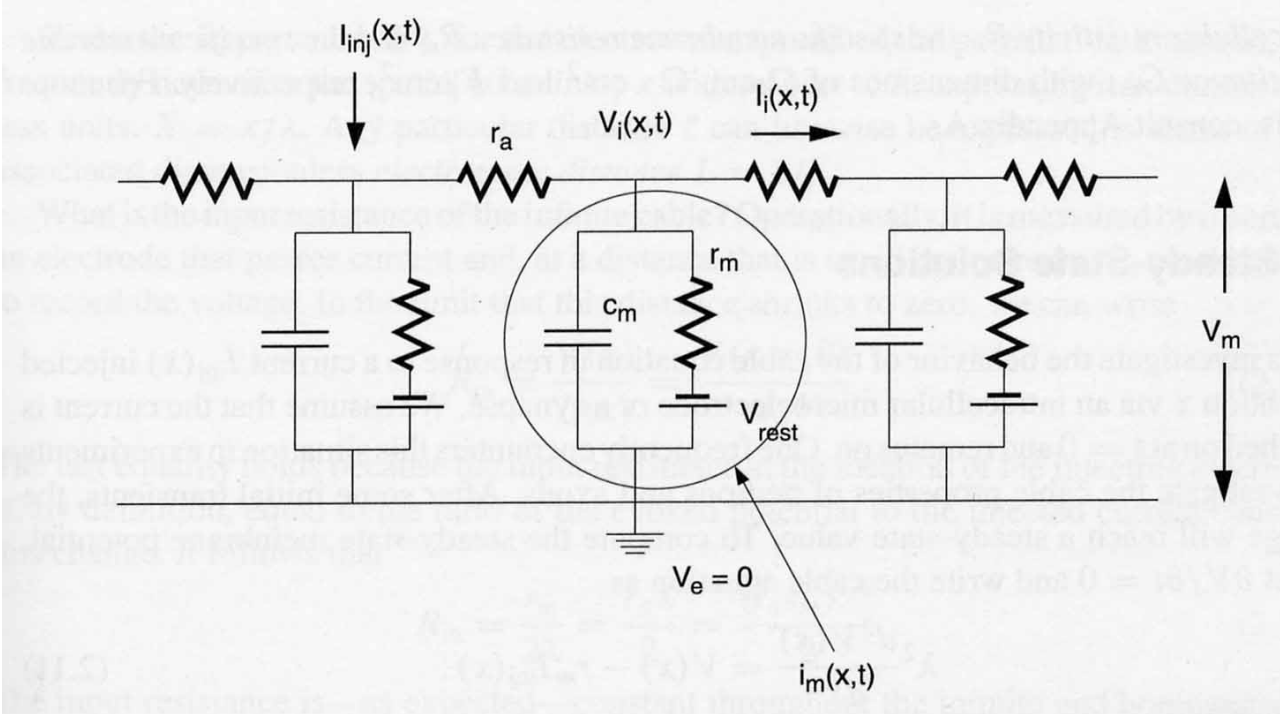


Fig. 2.3 A SINGLE PASSIVE CABLE Equivalent lumped electrical circuit of an elongated neuronal fiber with passive membrane. The intracellular cytoplasm is described by an ohmic resistance per unit length r_a and the membrane by a capacitance c_m in parallel with a passive membrane resistance r_m and a battery V_{rest}. The latter two components are frequently referred to as *leak resistance* and *leak battery*. An external current $I_{\text{inj}}(x,t)$ is injected into the cable. The associated linear cable equation (Eq. 2.7) describes the dynamics of the electrical potential $V_m = V_i - V_e$ along the cable.

Christof Koch, Biophysics of Computation. Information Processing in single neurons. Oxford University Press, New York 1999.

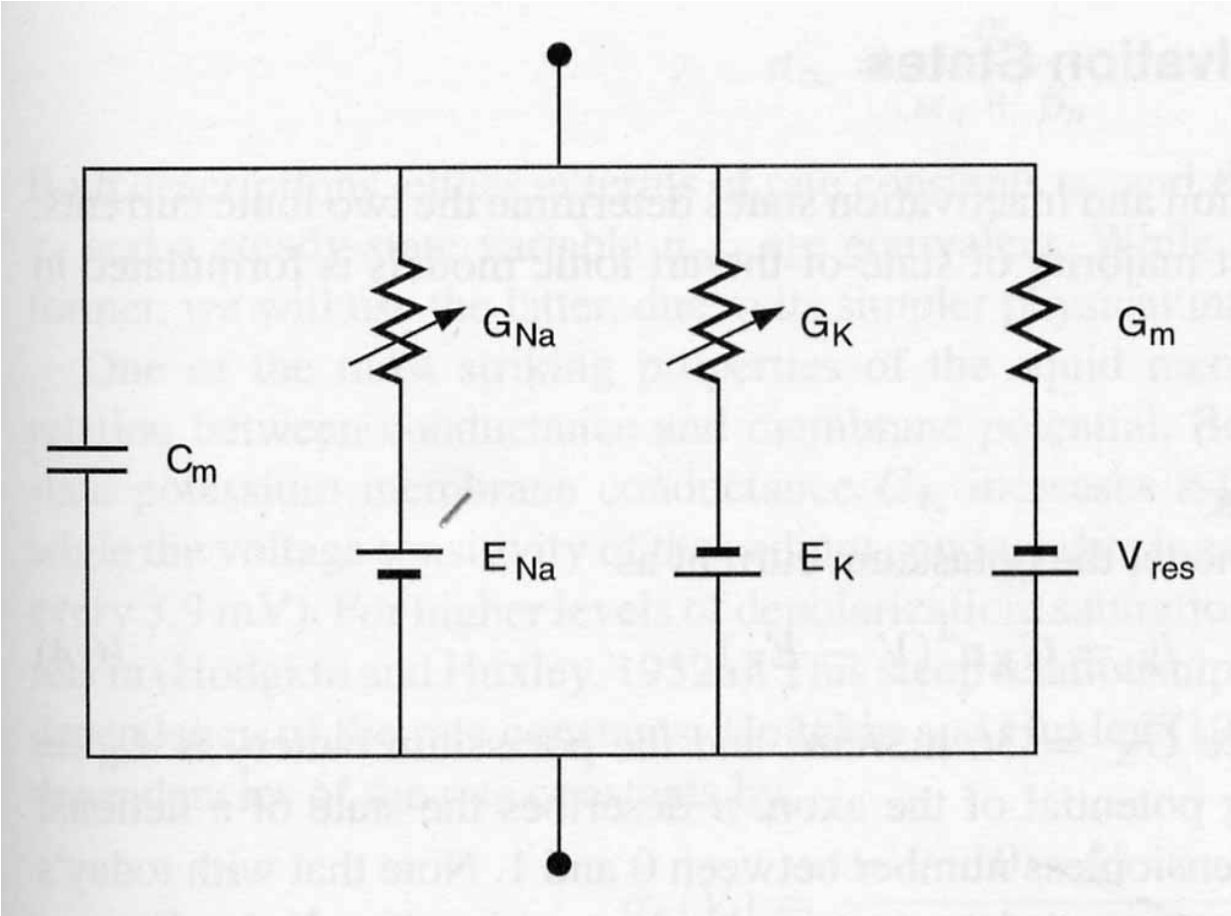


Fig. 6.2 Electrical Circuit for a Patch of Squid Axon Hodgkin and Huxley modeled the membrane of the squid axon using four parallel branches: two passive ones (membrane capacitance C_m and the leak conductance $G_m = 1/R_m$) and two time- and voltage-dependent ones representing the sodium and potassium conductances.

Christof Koch, Biophysics of Computation. Information Processing in single neurons. Oxford University Press, New York 1999.

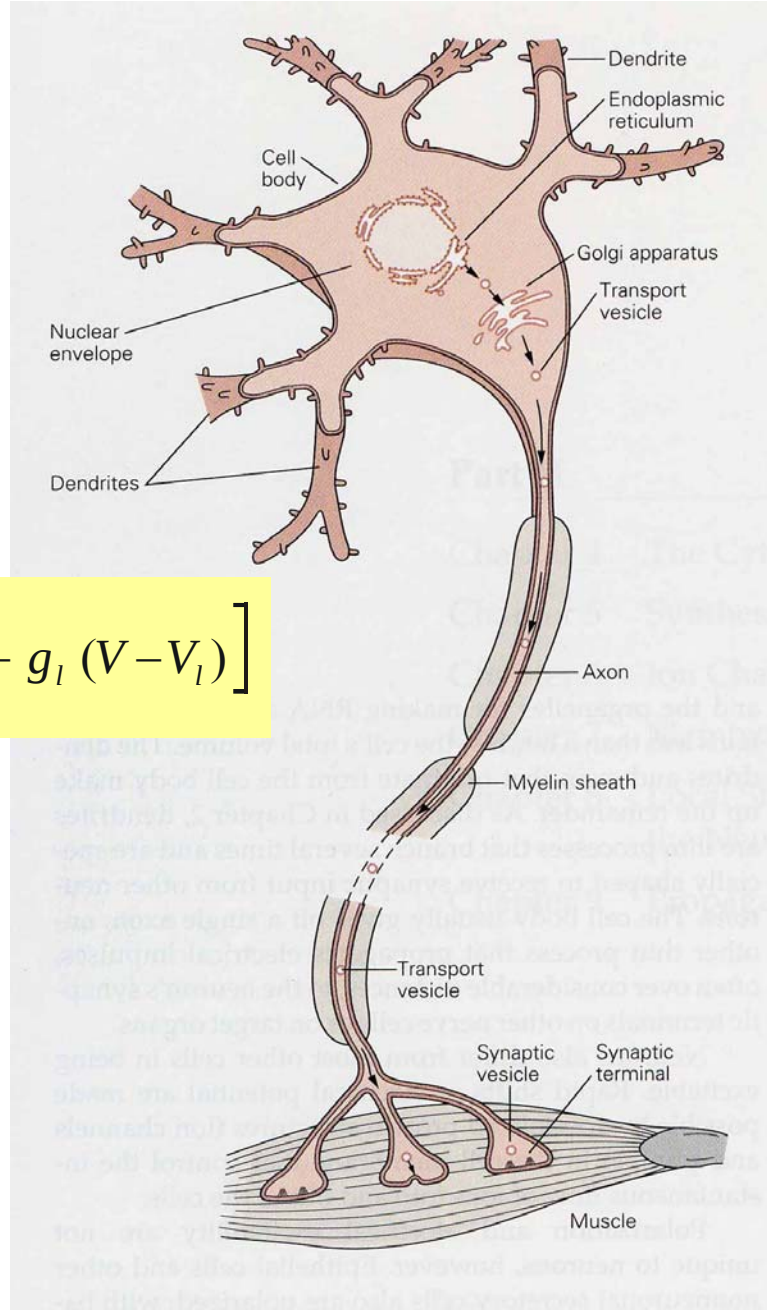
Hogdkin-Huxley OD equations

$$\frac{dV}{dt} = \frac{1}{C_M}\left[I - g_{Na}\, m^3\, h\,(V - V_{Na}) - g_K\, n^4\,(V - V_K) - g_l\,(V - V_l)\right]$$

$$\frac{dm}{dt} = \alpha_m\,(1-m) - \beta_m\, m$$

$$\frac{dh}{dt} = \alpha_h\,(1-h) - \beta_h\, h$$

$$\frac{dn}{dt} = \alpha_n\,(1-n) - \beta_n\, n$$



A single neuron signaling to a muscle fiber

$$\alpha_m = \frac{x}{e^x - 1}, \quad x = \frac{25 - V}{10} \; ; \quad \beta_m = 4 \exp\left[- \frac{V}{18} \right]$$

$$\alpha_h = 0.07 \exp\left[- \frac{V}{20} \right] \; ; \quad \beta_h = \frac{1}{e^x - 1}, \quad x = \frac{30 - V}{10}$$

$$\alpha_n = \frac{x}{10(e^x - 1)}, \quad x = \frac{10 - V}{10} \; ; \quad \beta_n = 0.125 \exp\left[- \frac{V}{80} \right]$$

Gating functions of the Hodgkin-Huxley equations

$$\frac{\partial m}{\partial t} = \Theta(T)\big[\alpha_m(1-m) - \beta_m m\big]$$

$$\frac{\partial h}{\partial t} = \Theta(T)\big[\alpha_h(1-h) - \beta_h h\big]$$

$$\frac{\partial n}{\partial t} = \Theta(T)\big[\alpha_n(1-n) - \beta_n n\big] \ ,$$

$$\text{where } \ \Theta(T) = 3^{(T-6.3)/10}$$

Temperature dependence of the Hodgkin-Huxley equations

$$\frac{dV}{dt} = \frac{1}{C_M}\left[I - \bar{g}_{Na}\, m^3\, h\,(V - V_{Na}) - \bar{g}_K\, n^4\,(V - V_K) - \bar{g}_l\,(V - V_l)\right]$$

$$\frac{dm}{dt} = \alpha_m\,(1-m) - \beta_m\, m$$

$$\frac{dh}{dt} = \alpha_h\,(1-h) - \beta_h\, h$$

$$\frac{dn}{dt} = \alpha_n\,(1-n) - \beta_n\, n$$

Hogdkin-Huxley OD equations

Hhsim (2).lnk

Simulation of space independent Hodgkin-Huxley equations:
Voltage clamp and constant current

$$\frac{1}{R}\frac{\partial^2 V}{\partial x^2} = C\frac{\partial V}{\partial t} + \left[g_{Na}\, m^3\, h (V - V_{Na}) + g_K\, n^4\, (V - V_K) + g_l\, (V - V_l) \right] 2\pi\, r\, L$$

$$\frac{\partial m}{\partial t} = \alpha_m (1 - m) - \beta_m\, m$$

$$\frac{\partial h}{\partial t} = \alpha_h (1 - h) - \beta_h\, h$$

$$\frac{\partial n}{\partial t} = \alpha_n (1 - n) - \beta_n\, n$$

Hodgkin-Huxley PDEquations

Travelling pulse solution: $V(x,t) = V(\xi)$ with

$$\xi = x + \theta\, t$$

Hodgkin-Huxley equations describing pulse propagation along nerve fibers

$$\frac{1}{R}\frac{d^2V}{d\xi^2} = C_M\,\theta\frac{dV}{d\xi} + \left[\,\bar{g}_{Na}\,m^3\,h(V-V_{Na}) + \bar{g}_K\,n^4\,(V-V_K) + \bar{g}_l\,(V-V_l)\right]\,2\pi r L$$

$$\theta\,\frac{dm}{d\xi} = \alpha_m\,(1-m) - \beta_m\,m$$

$$\theta\,\frac{dh}{d\xi} = \alpha_h\,(1-h) - \beta_h\,h$$

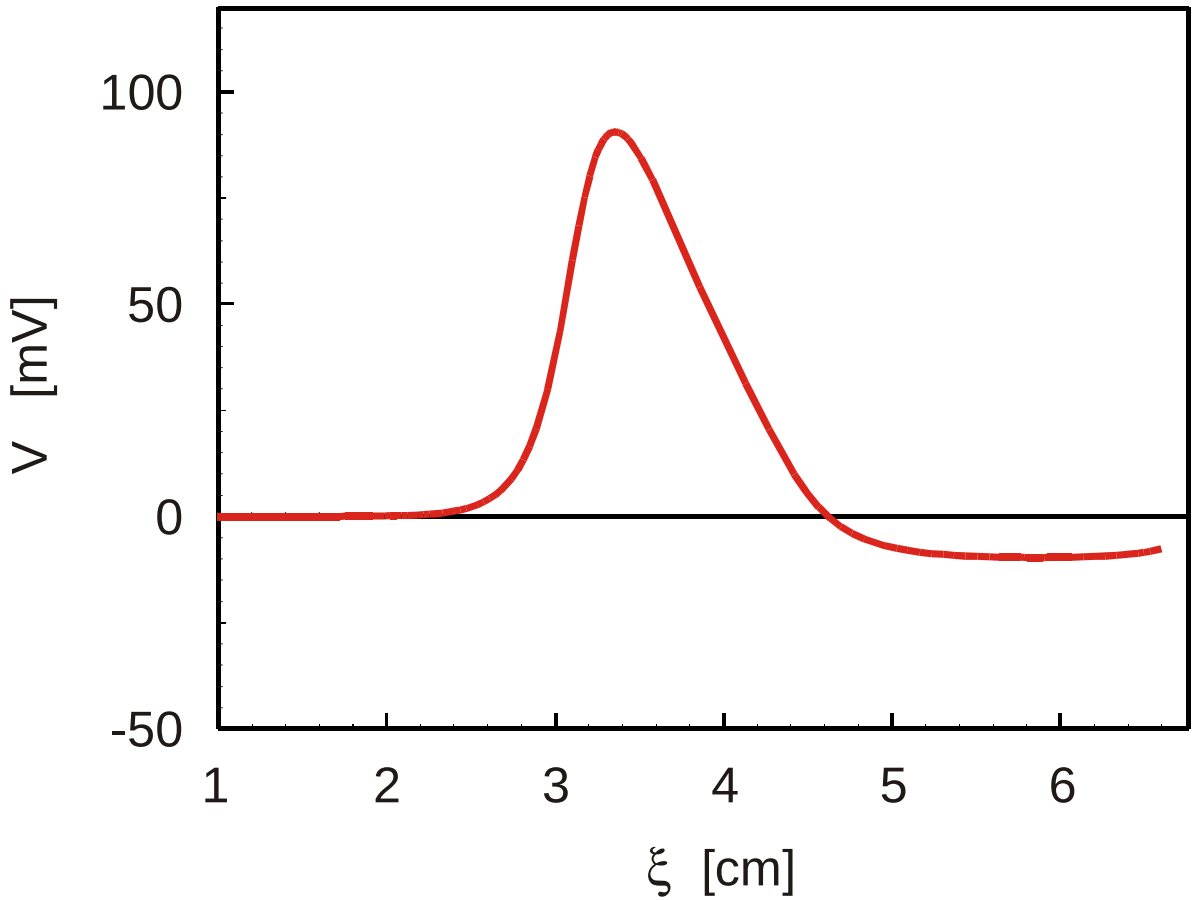
$$\theta\,\frac{dn}{d\xi} = \alpha_n\,(1-n) - \beta_n\,n$$

Hodgkin-Huxley PDEquations

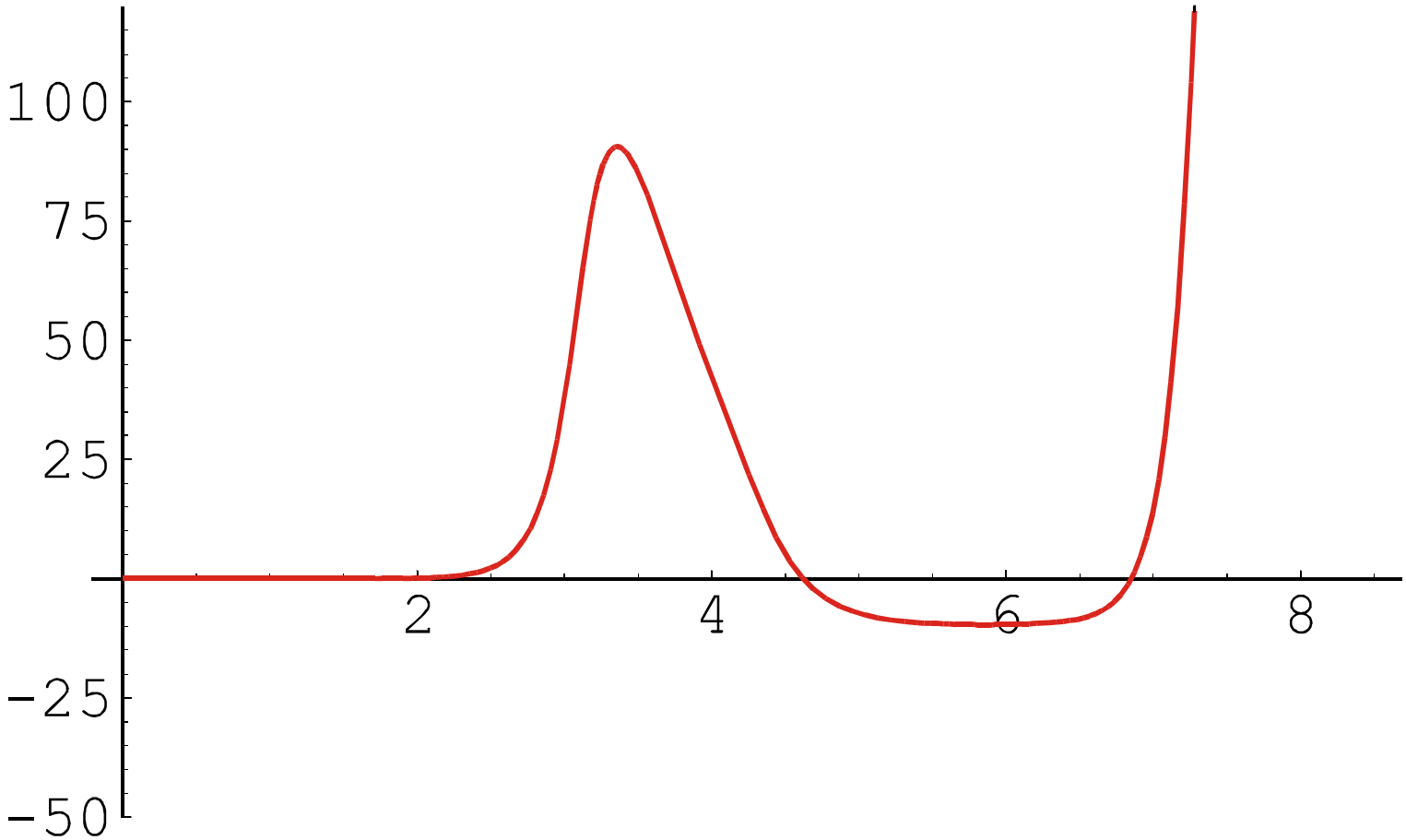
Travelling pulse solution: $V(x,t) = V(\xi)$ with

$$\xi = x + \theta\,t$$

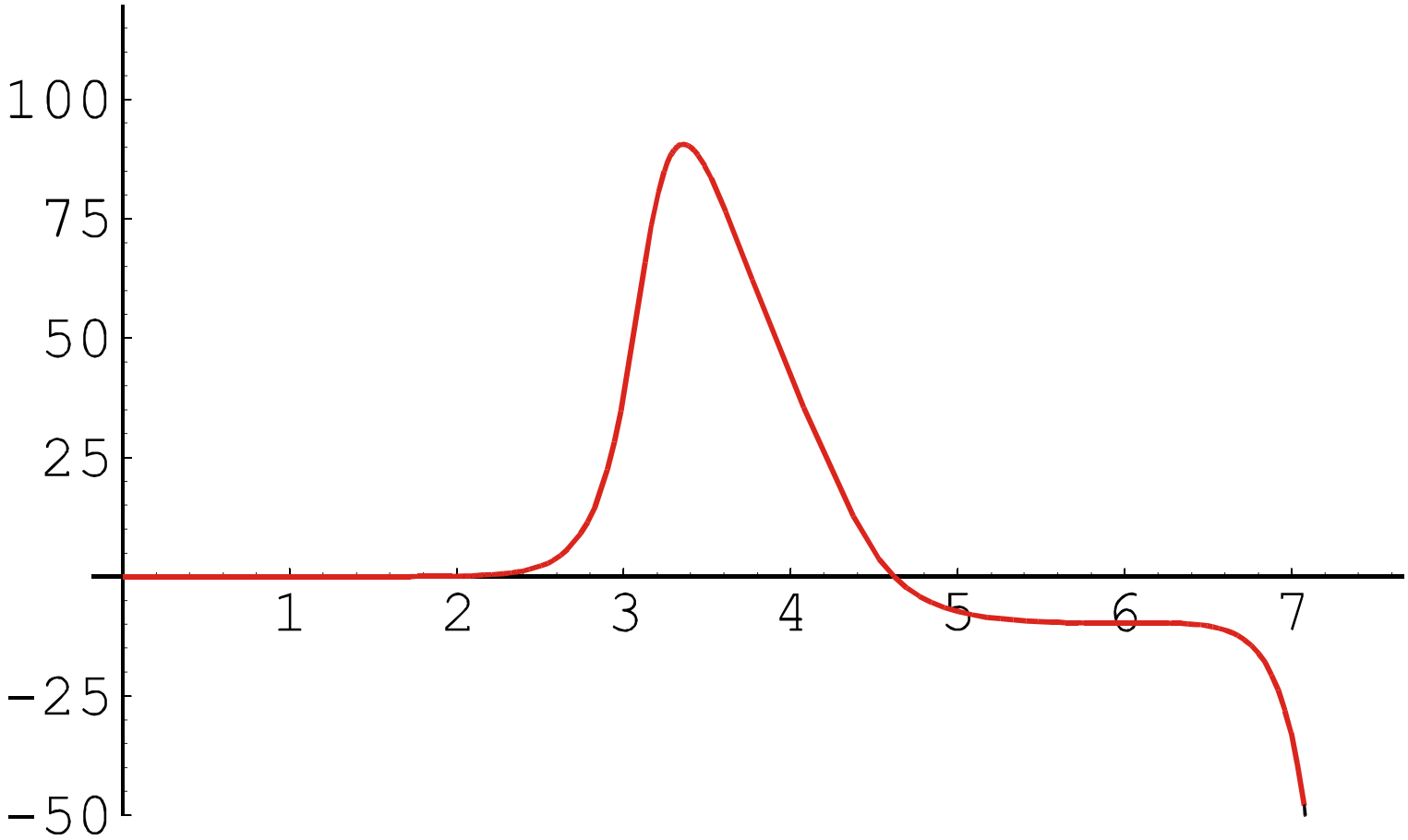
Hodgkin-Huxley equations describing pulse propagation along nerve fibers



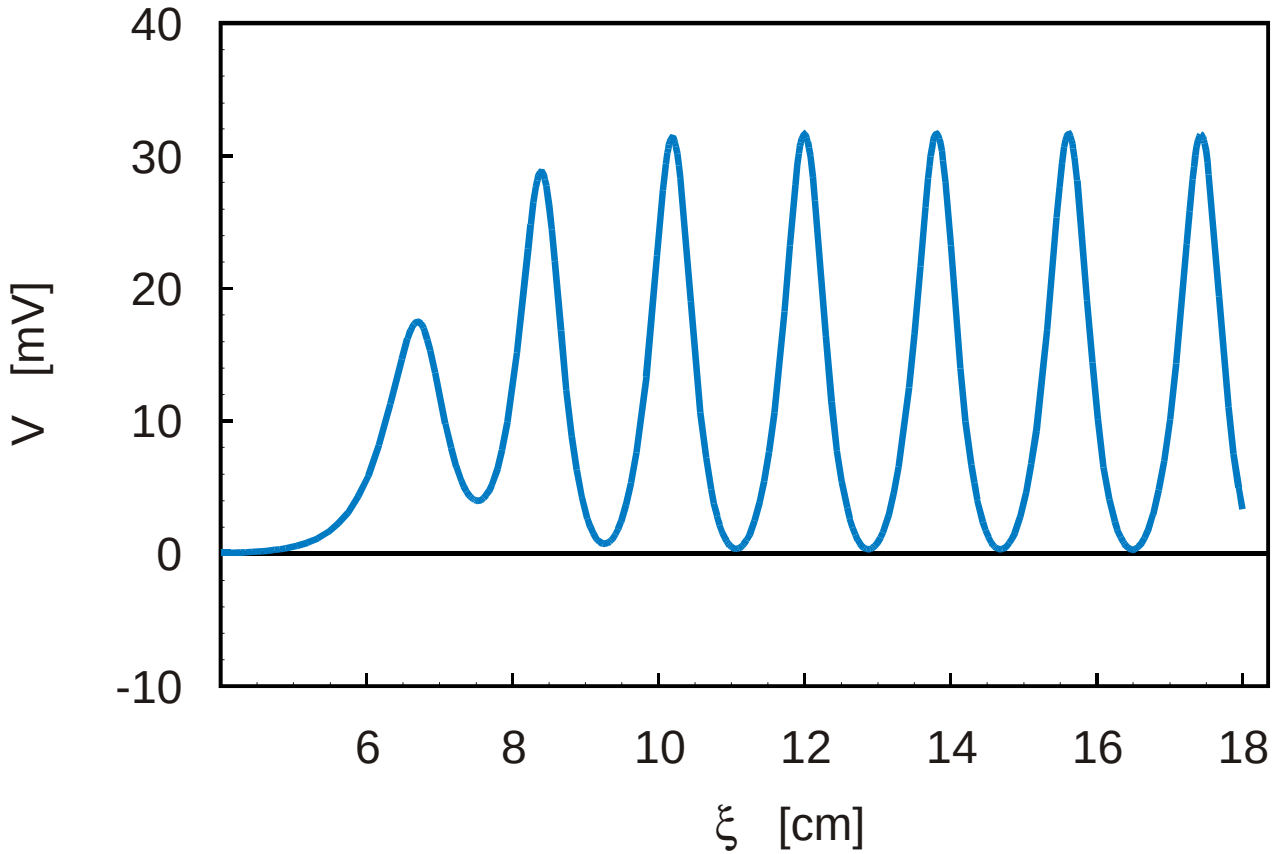
T = 18.5 C; θ = 1873.33 cm / sec



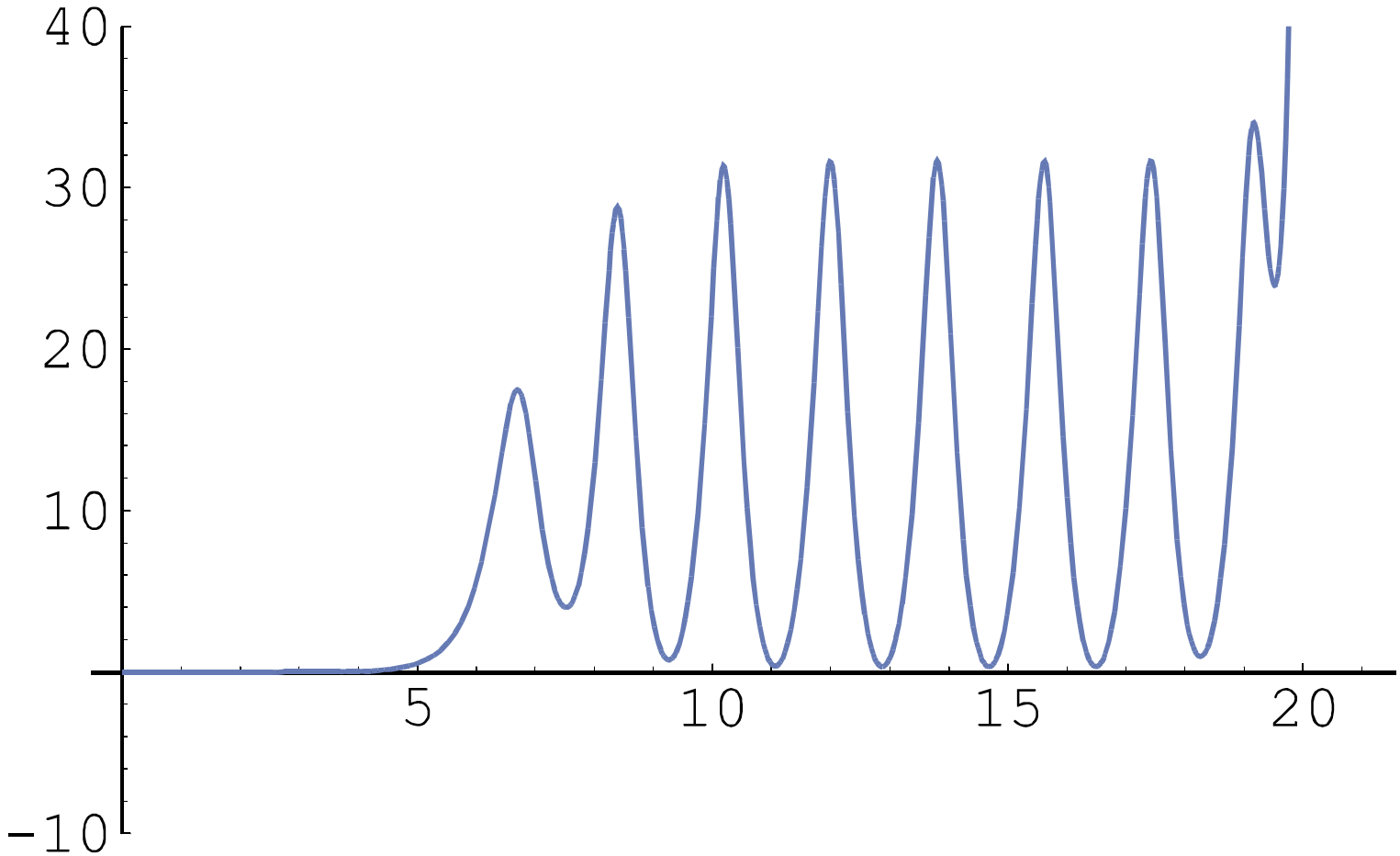
T = 18.5 C; θ = 1873.3324514717698 cm / sec



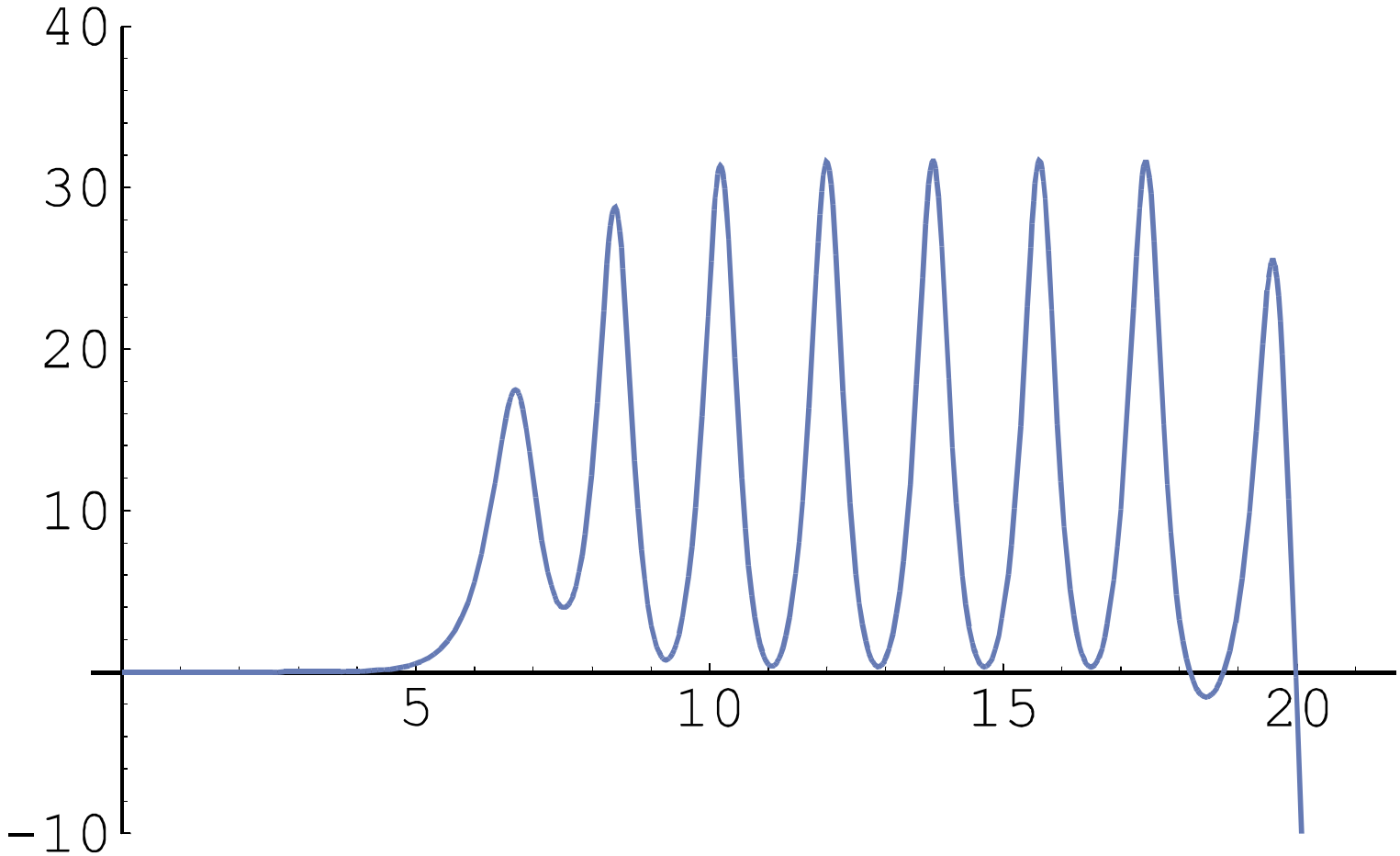
T = 18.5 C; θ = 1873.3324514717697 cm / sec



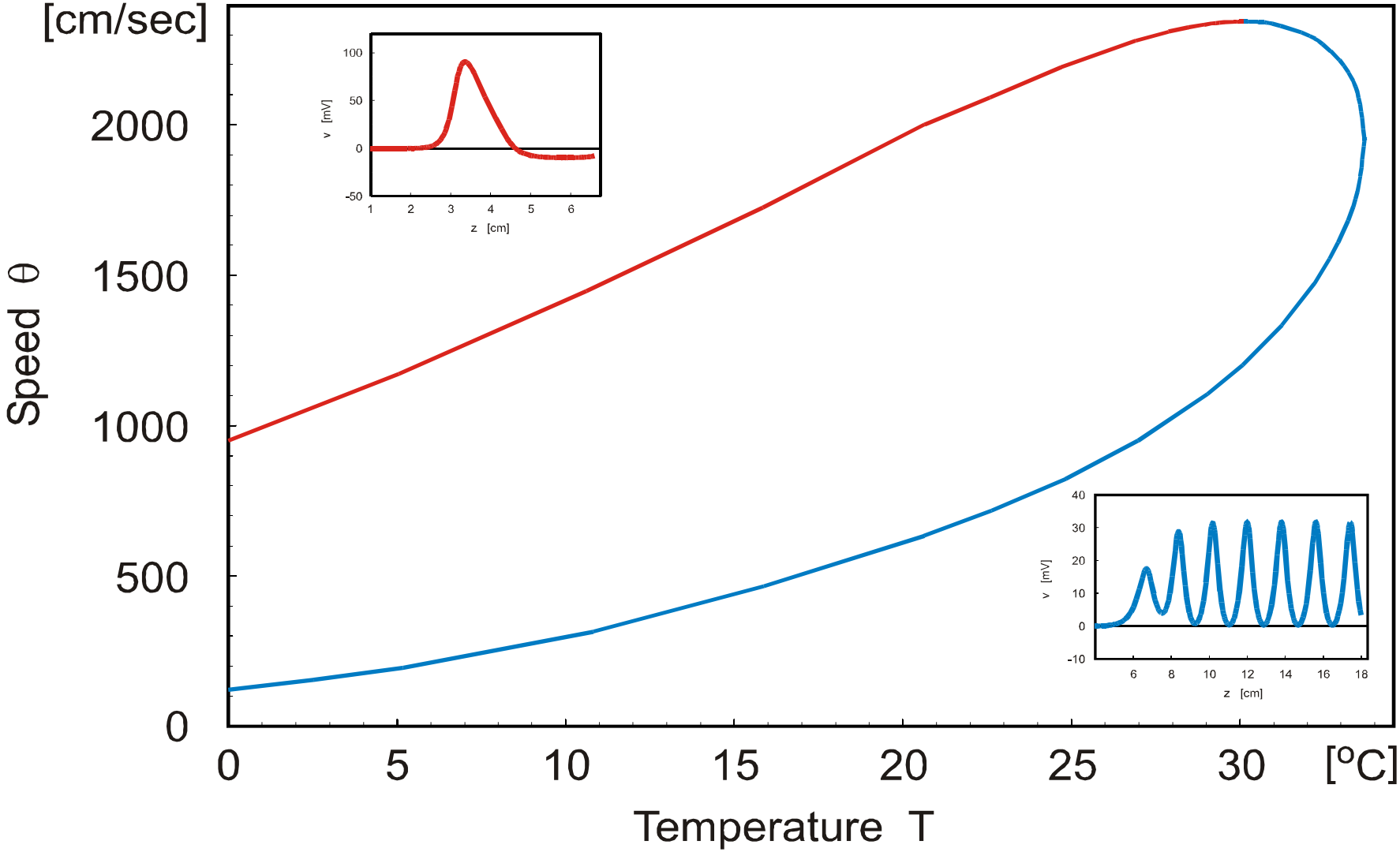
T = 18.5 C; θ = 544.070 cm / sec



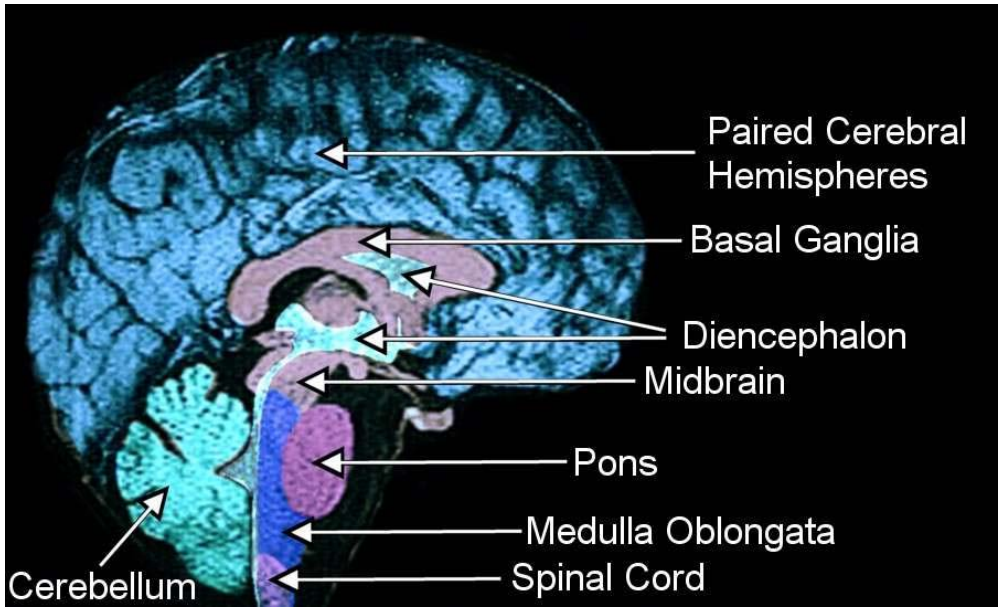
T = 18.5 C; θ = 554.070286919319 cm/sec

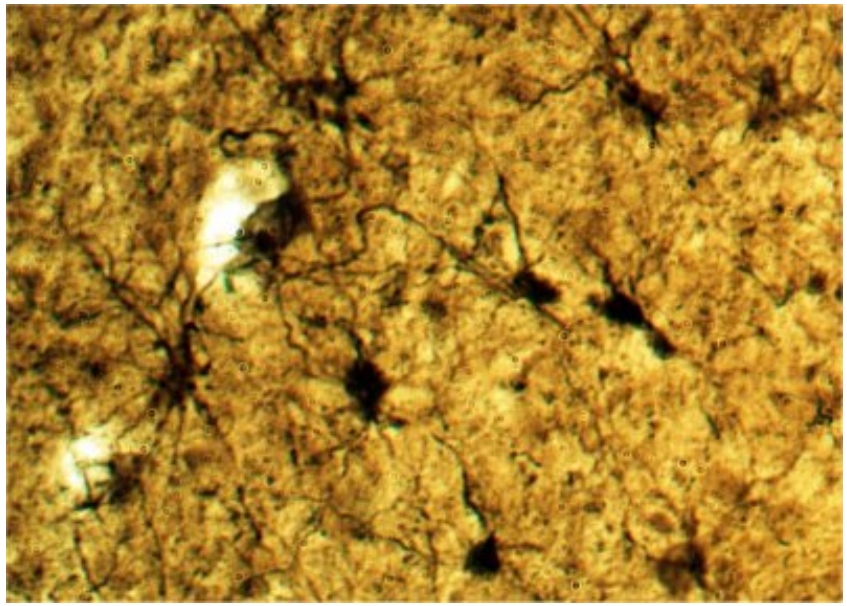


T = 18.5 C; θ = 554.070286919320 cm/sec



Propagating wave solutions of the Hodgkin-Huxley equations





The human brain

10^{11} neurons connected by $\approx 10^{13}$ to 10^{14} synapses

Universität Wien

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