

The influence of time irreversibility on the stability of material systems.

Science is built up of facts, as a house is with stones. But a collection of facts is no more a science than a heap of stones is a house.

Henri Poincaré

*An open, growing system evolves and stays stable.
A closed system tends toward equilibrium — and is biologically dead.*

Evolution

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The location of living matter in universe.

Competition between gravitational and electromagnetic forces

The ratio of interacting forces between H^+ and e^- :

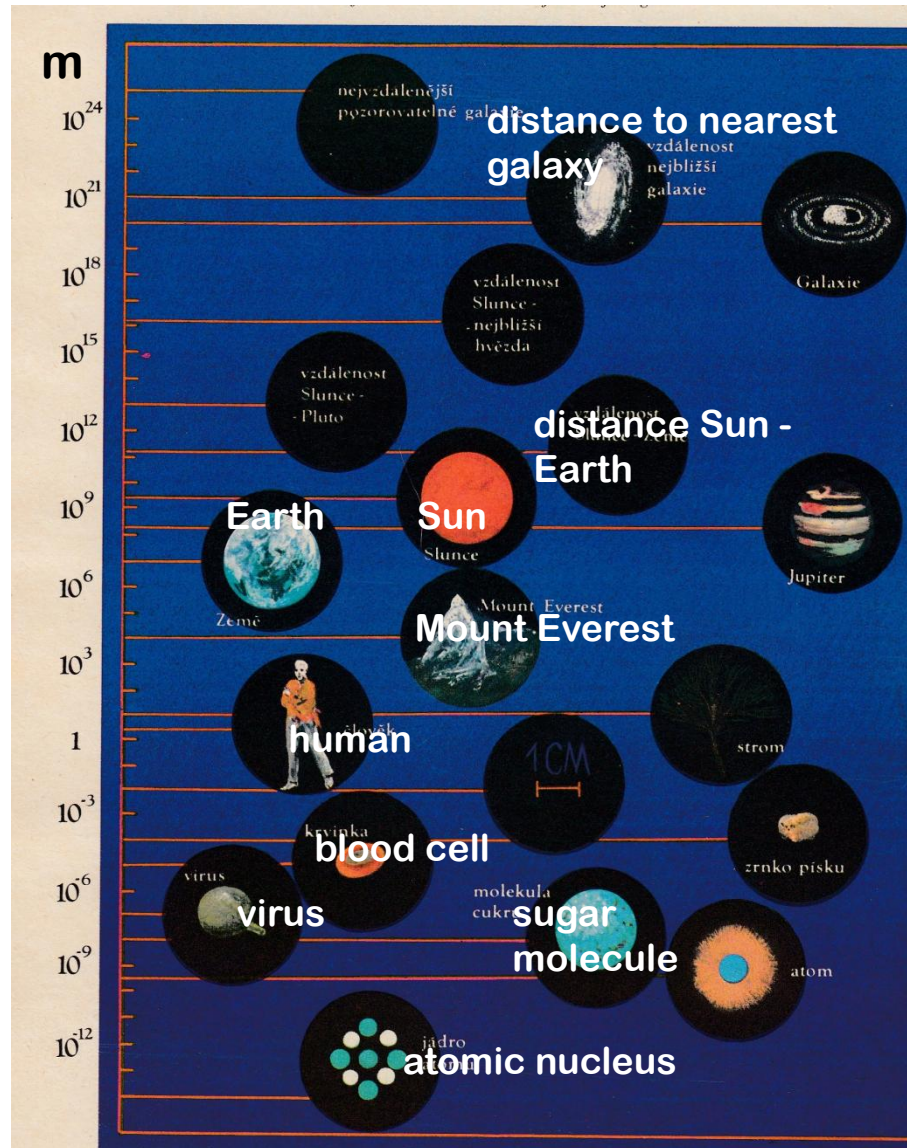
$$\frac{F_{elmag}}{F_{gravi}} = \frac{\frac{q_{e^-} q_{H^+}}{4\pi\epsilon_0 r^2}}{G \frac{m_{e^-} m_{H^+}}{r^2}} = \frac{2.3 \cdot 10^{-28}}{1.01 \cdot 10^{-67}} = 2.3 \cdot 10^{39}$$

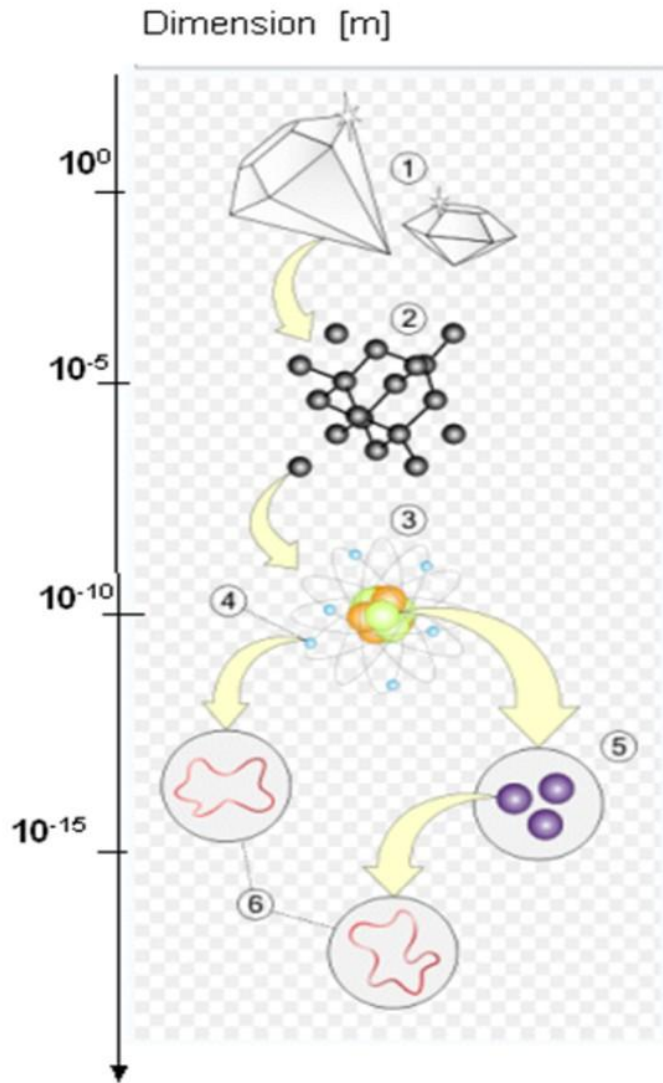
Object size ratio

$$\frac{\text{observable universe}}{\text{Bohr's radius}} = \frac{8.8 \cdot 10^{26}}{5.3 \cdot 10^{-11}} = 1.6 \cdot 10^{37}$$

Due to the closeness of these ratios, it is clear that the structure of the universe is controlled by the gravitational force and the structure of living matter by the electromagnetic force.

Distances/sizes of objects in the Universe

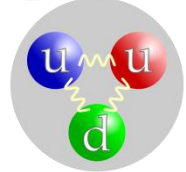




Levels of magnification:

1. Macroscopic level - Matter
2. Molecular level
3. Atomic level - Protons, neutrons, and electrons
4. Subatomic level - Electron
5. Subatomic level - Quarks
6. String level -- possible

proton



Three Generations of Matter (Fermions)

	I	II	III	
mass	3 MeV	1.24 GeV	172.5 GeV	0
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
name	u up	c charm	t top	γ photon
	6 MeV	95 MeV	4.2 GeV	0
Quarks	$-\frac{1}{3}$ $\frac{1}{2}$ d down	$-\frac{1}{3}$ $\frac{1}{2}$ s strange	$-\frac{1}{3}$ $\frac{1}{2}$ b bottom	0 1 g gluon
	<2 eV	<0.19 MeV	<18.2 MeV	~126 GeV/c ² 0 0 H Higgs boson
	0 $\frac{1}{2}$ ν_e electron neutrino	0 $\frac{1}{2}$ ν_μ muon neutrino	0 $\frac{1}{2}$ ν_τ tau neutrino	90.2 GeV 0 1 Z ⁰ weak force
Leptons	0.511 MeV -1 $\frac{1}{2}$ e electron	106 MeV -1 $\frac{1}{2}$ μ muon	1.78 GeV -1 $\frac{1}{2}$ τ tau	80.4 GeV ± 1 1 W [±] weak force
				Bosons (Forces)

Standard_Model_of_Elementary_Particles.svg (SVG file, nominally 600 × 650 pixels, file size: 26 KB)

$$l_{\text{Planck}} = \sqrt{\hbar G_N / c^3} \approx 1.616 \cdot 10^{-35} \text{ m}$$

the dimension of the smallest object in the universe

Time direction

I. the time of human consciousness – a sequence of experiences

becoming → being

II. time in biology – parameter of development,

birth → death

thermodynamics – impossibility of returning to the initial state

(non-invariance with respect to $t \rightarrow -t$)

e.g., for heat conduction $\frac{\partial T}{\partial t} = a \Delta T, \Rightarrow$ Entropy production $P(S) = \frac{\lambda}{T^2} (\nabla T)^2 \geq 0$

III. time of theoretical physics - parameter of change

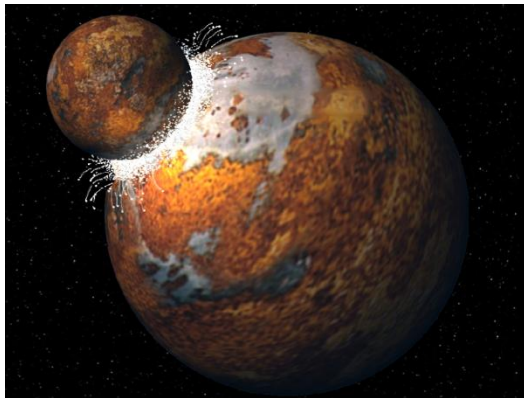
For conservative systems $\frac{\partial H(p_i(t), q_i(t))}{\partial t} = 0, \dot{p}_i(t_0, t) = -\frac{\partial H}{\partial q_i} \Rightarrow F_i(q_j),$

$$\dot{q}_i(t_0, t) = \frac{\partial H}{\partial p_i} \Rightarrow v_i(t_0, t) \text{ for } i, j = 1, 2, \dots, N$$

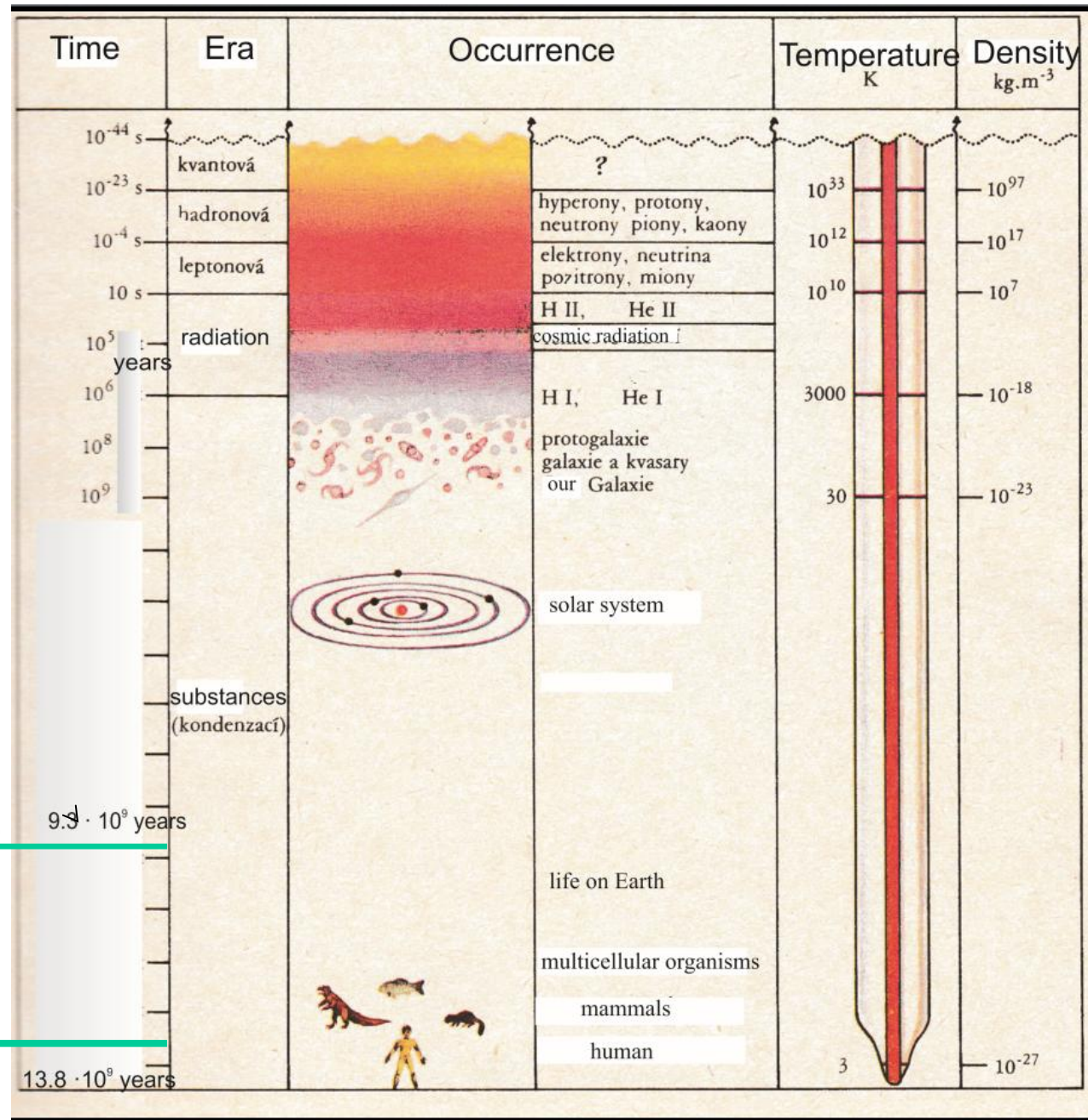
(invariance with respect to time reversibility, i.e., $t \rightarrow -t$)

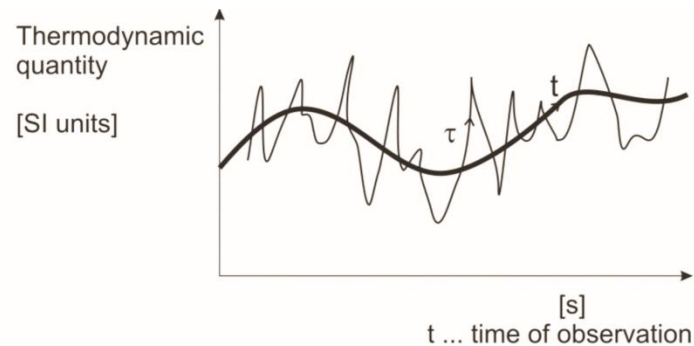
The beginning of the universe
--the evolution of the universe in time

The collision of the THEIA
with the Earth—the formation
of the moon

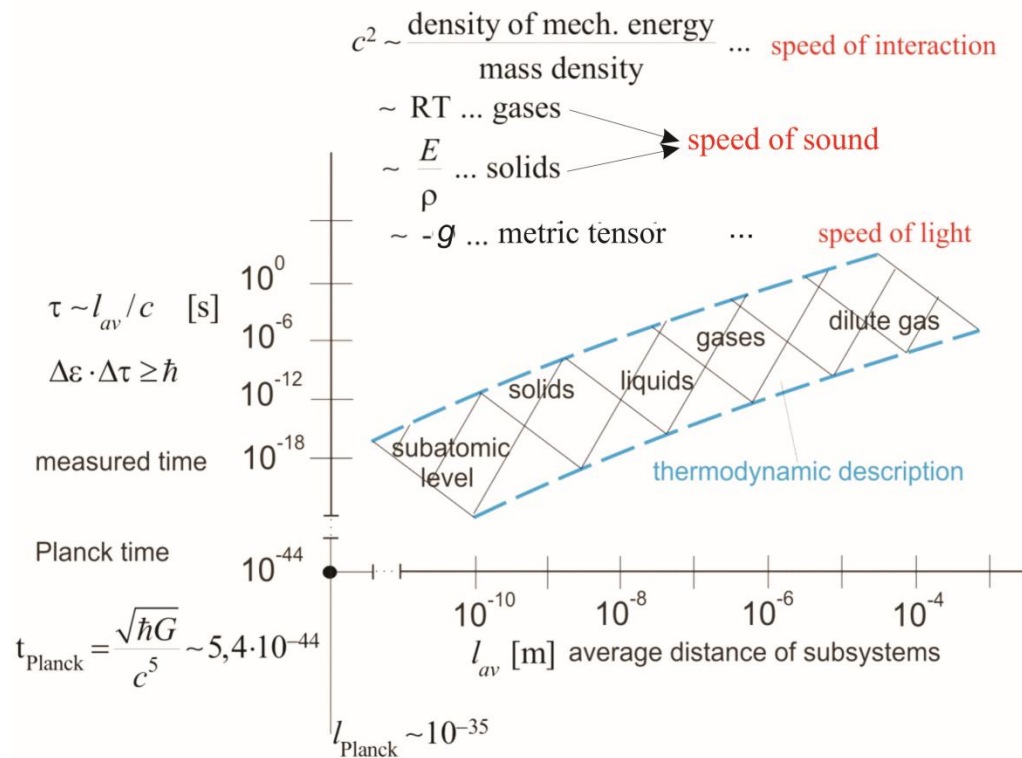


Giant asteroid caused
extinction of dinosaurs
66 million years ago

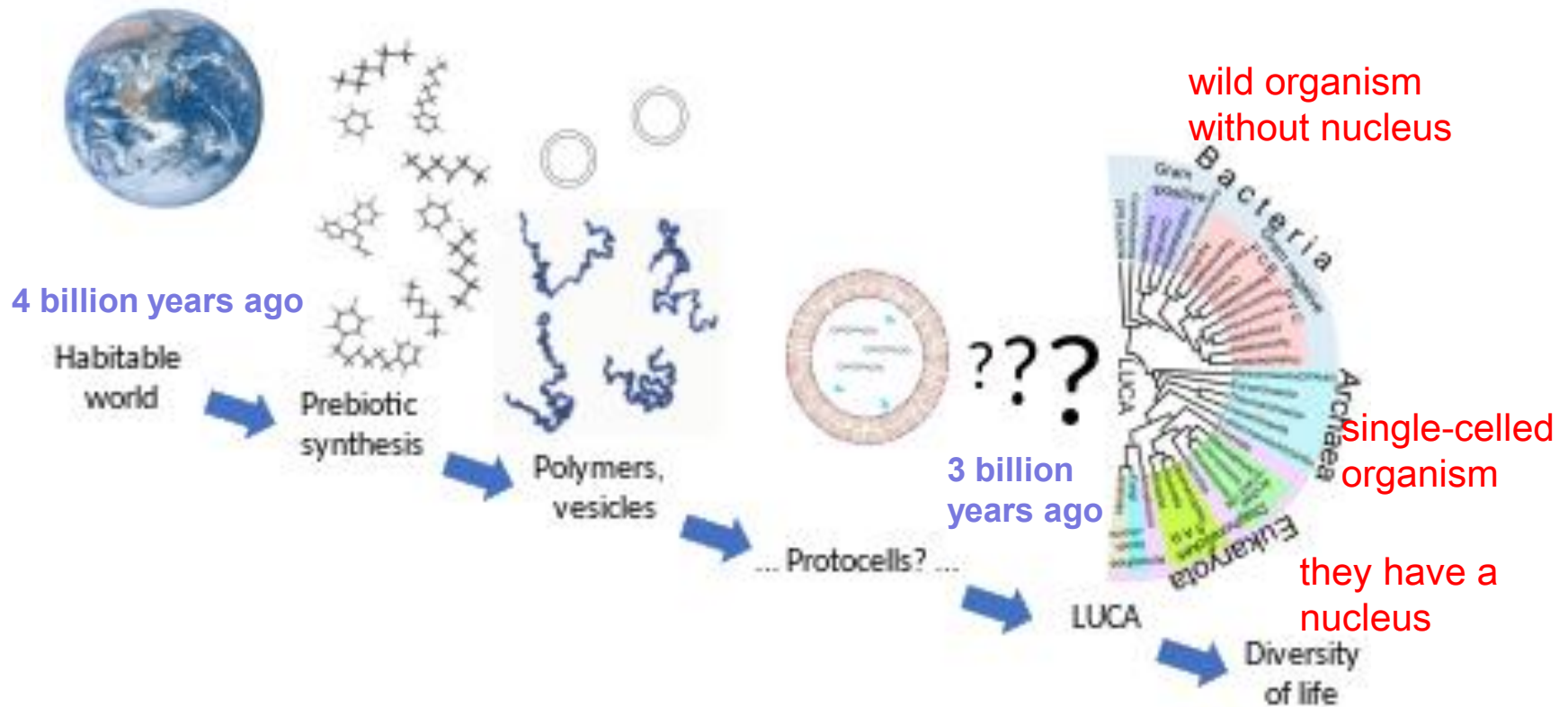




t ... time of fluctuation - mean interaction time
for macroscopic (thermodynamic) description is needed $d\tau \ll dt$



Evolution is the change in the hereditary characteristics of biological populations over successive generations.



The last universal common ancestor (LUCA) is the last population from which all organisms now living on Earth share a common origin.

<https://en.wikipedia.org/wiki/Evolution>

Nowadays, thermodynamics is understood as a physical discipline that starts from the general laws of the transformation of energy and matter and draws consequences from them.

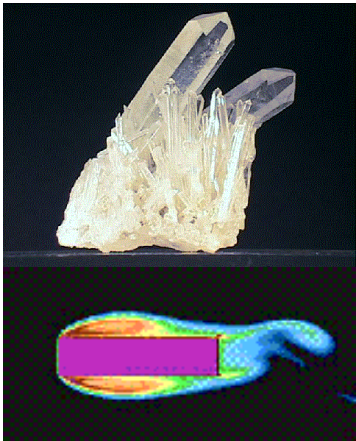
(dialectic of MATTER and FIELD)

It investigate real bodies - thermodynamic systems (hereafter referred to as systems), **which consist of a large number of mutually acting (interacting) parts** - subsystems (e.g. atoms, molecules, etc.). Examples from everyday life: solid body, liquids, biological individual or part thereof, ecological system, etc.

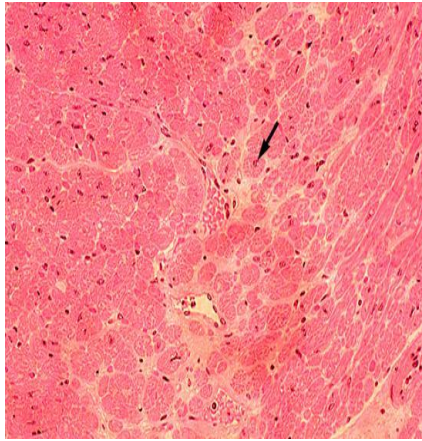
By interaction we mean all known ways of mutual influence between bodies and their parts in nature. It mainly concerns the exchange of all forms of energy, momentum and matter.

Examples of open systems

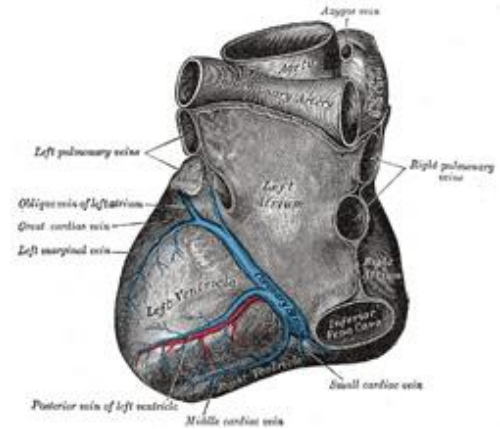
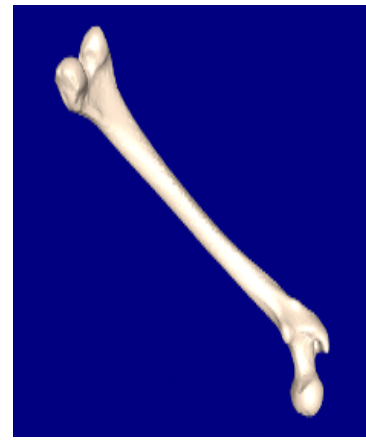
Solids and fluids



Living cells - blood



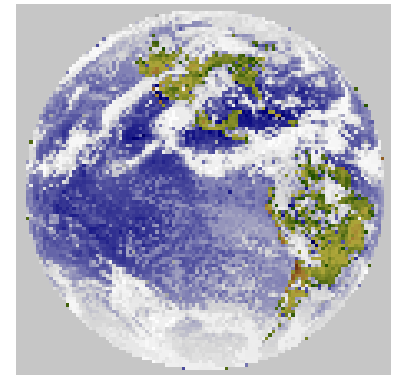
Living tissue



Animals and human being



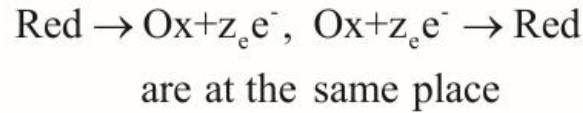
EARTH



Evolution in energy transformation

$$\Delta W_{\text{exp}} = 0, \Delta S > 0$$

$$\underbrace{\Delta W_{\text{exp}}}_{p\Delta V} = \underbrace{T\Delta S}_{\Delta Q \cdots \text{combustion}} - \Delta U \xrightarrow{T=\text{const}} -\Delta F$$



$$\Delta W_{\text{exp}} > 0, \Delta S > 0$$



$$\Delta Q = T\Delta S \stackrel{\text{steady}}{=} \Delta H_{\text{tot}} = \Delta H + \Delta W_{\text{pot}} + \Delta W_{\text{kin}} > 0$$

$$\Delta H \approx 0$$

$$\Delta W_{\text{kin}} \rightarrow \Delta W_e,$$

$$\Delta S \rightarrow 0$$



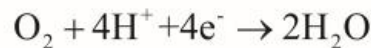
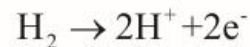
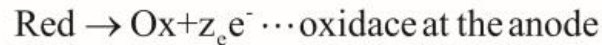
$$\Delta W_{\text{kin}} \rightarrow \Delta W_e,$$

$$\Delta S \rightarrow 0$$



$$\underbrace{\Delta W_{\text{non-exp}}}_{V\Delta p + W_e} = T\Delta S - \Delta H = \xrightarrow[\text{semiconductor or polym. elektrol. membrane}]{T=\text{const}} - \underbrace{\Delta G}_{\text{chem. reaction, radiation}}$$

$$\Delta S > 0$$



$$W_e$$

$$\Delta S > 0$$



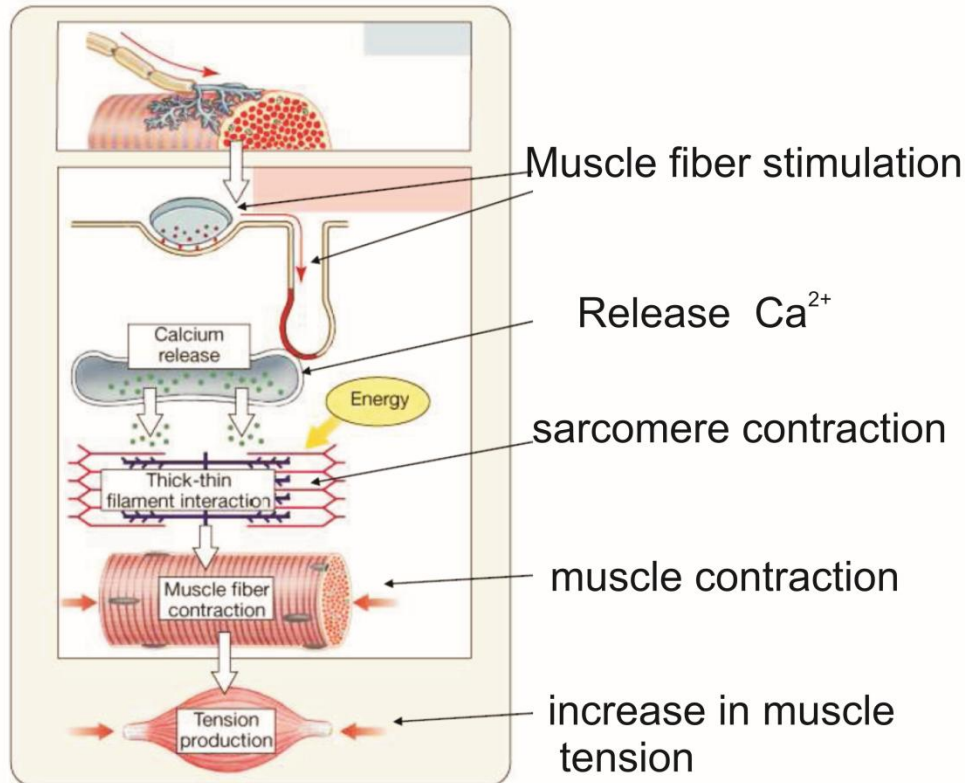
Muscle force generation --molecular motors

Mechanical tension in the muscle is induced by the reaction



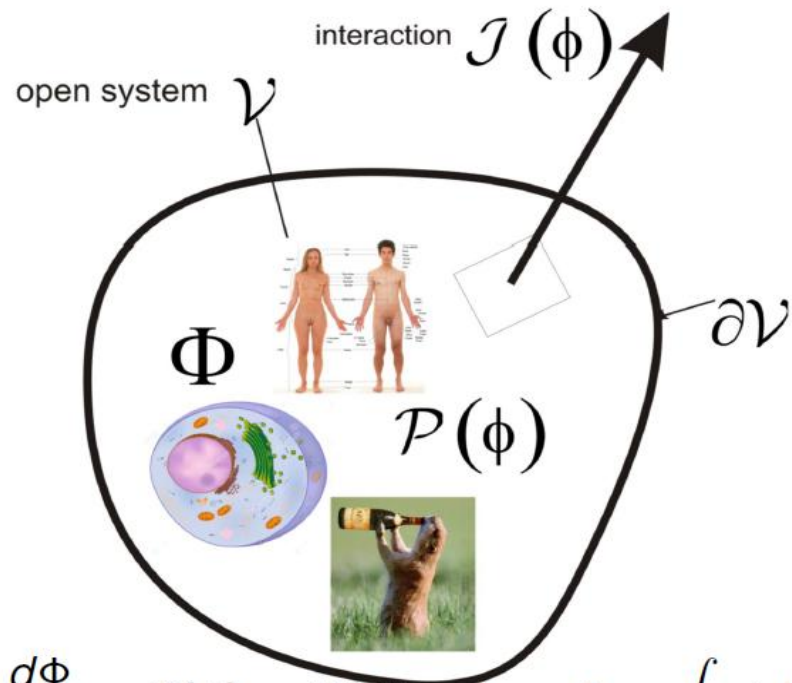
$$\Delta G = -30\text{kJ mol}^{-1}, \Delta H = -20\text{kJ mol}^{-1}, \Delta S = +34\text{J mol}^{-1}\text{K}^{-1}$$

Excitation and contraction



Time evolution of relevant quantities

Global form of the balance laws is



$$\frac{d\Phi}{dt} + \mathcal{J}(\phi) = \mathcal{P}(\phi), \quad \text{for } \Phi = \int_V \phi d\nu$$

This time change (d/dt) of the quantity Φ is caused by

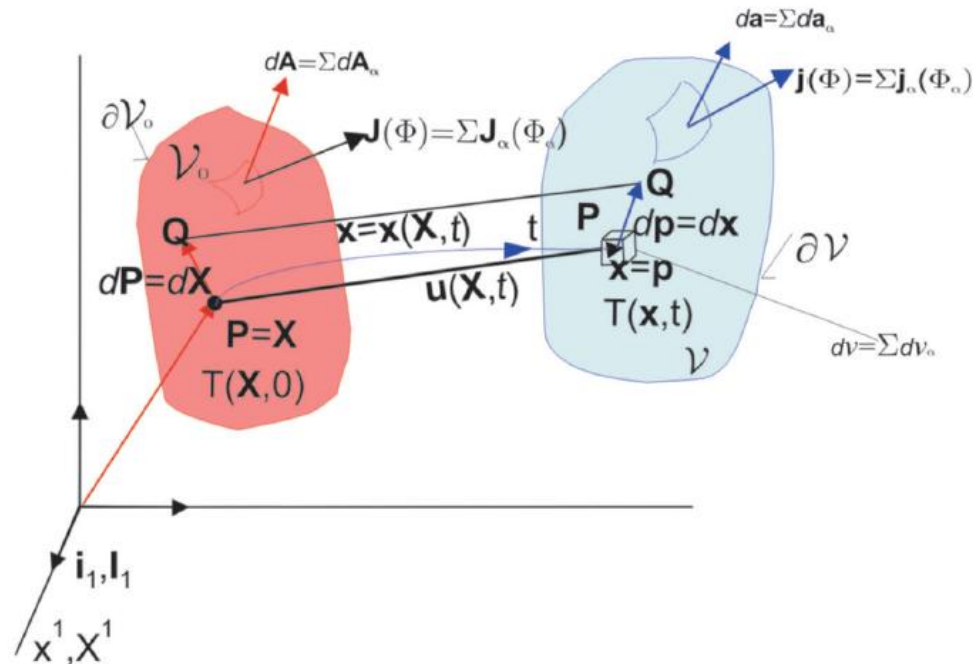
$$\mathcal{J}(\phi) = \int_{\partial V} \mathbf{j} d\mathbf{a} \quad \text{the flux through the boundary and}$$

$$\mathcal{P}(\phi) = \int_V \sigma(\phi) d\nu \quad \text{by the total production of this quantity } \phi$$

General form of balance laws

The change of the extensive quantity Φ in the body with volume $\mathcal{V}$ can be compensated by the flux $\mathcal{J}(\Phi)$ thorough the surface $\partial\mathcal{V}$ and/or by the production $\mathcal{P}(\Phi)$ in the body.

REFERENCE CONFIGURATION MATERIAL DESCRIPTION $(\mathbf{X}, t)$	ACTUAL CONFIGURATION SPACE DESCRIPTION $(\mathbf{x}, t)$
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Measured extensive quantities

All important measurable extensive quantities are defined by their **balance laws**. The convenient set of such quantities $\Phi(t)$ applied for the time evolution (physical description) of the real physical system, which occupied the volume $\mathcal{V}$, with the boundary $\partial\mathcal{V}$ have the following physical interpretation

$$\Phi = \left(\begin{array}{l} \rho_\alpha, \rho_m, \rho_e \\ D, B \\ \rho \\ \rho_\alpha v_\alpha, \rho v \\ \nabla \times \rho_\alpha v_\alpha, \nabla \times \rho v \\ \frac{\rho_\alpha v_\alpha^2}{2}, \frac{\rho v^2}{2} \\ \rho_\alpha u_\alpha, \rho u \\ \rho_\alpha s_\alpha, \rho s \end{array} \right) \begin{array}{l} \text{-chem. components, el. and mag. charges} \\ \text{- electric and magnetic inductions fields} \\ \text{-mass} \\ \text{- momentum} \\ \text{- momentum of momentum} \\ \text{- mechanical energy} \\ \text{- internal energy} \\ \text{- entropy} \end{array}$$

Balance of total energy I. Law of Thermodynamics

Balance of internal energy U of the system occupying the time-varying volume $\mathcal{V}$ with surface $\partial\mathcal{V}$ follows from the balance of total energy. For homogeneous one component system we have

$$\dot{U} - \dot{Q} = \int_{\mathcal{V}} \left[(\mathbf{t}_{el} + \mathbf{t}_{dis}) : \nabla \mathbf{v} + \mathbf{j}_e \mathbf{E} + \rho \mathbf{E} \left(\frac{\dot{\mathbf{P}}}{\rho} \right) + \rho \mathbf{B} \left(\frac{\dot{\mathbf{M}}}{\rho} \right) \right] d\nu + \dot{Q}^{EX} \quad (2.1)$$

$$\rho \dot{u} = -\text{div} \mathbf{j}_q + \mathbf{t} : \nabla \mathbf{v} + \mathbf{j}_e \mathbf{E} + \rho \mathbf{E} \left(\frac{\dot{\mathbf{P}}}{\rho} \right) + \rho \mathbf{B} \left(\frac{\dot{\mathbf{M}}}{\rho} \right) + q^{ex}$$

For the multicomponent system of density $\rho = \sum_{\alpha} \rho_{\alpha}$ composed from chemically reacting components we start with an alternative form of the balance of energy

$$\rho \dot{u} + \text{div} \left(\mathbf{j}_q + \sum_{\alpha} \mathbf{j}_{D_{\alpha}} u_{\alpha} - \frac{\mathbf{j}_{D_{\alpha}} \cdot \mathbf{t}_{\alpha}}{\rho} \right) = \mathbf{t} : \nabla \mathbf{v} - \sum_{\alpha} \rho_{\alpha} \mathbf{v}_{D_{\alpha}} \otimes \mathbf{v}_{D_{\alpha}} : \nabla \mathbf{v} \quad (2.2)$$

$$+ \sum_{\alpha} \mathbf{j}_{D_{\alpha}} \cdot (\mathbf{b}_{\alpha} + \mathbf{\Gamma}_{\alpha}) - \sum_{\alpha} \rho \omega_{\alpha} (\phi_{\alpha} + \gamma_{\alpha})$$

for $u = \sum_{\alpha} w_{\alpha} u_{\alpha}$, $w_{\alpha} = \frac{\rho_{\alpha}}{\rho}$, $\omega_{\alpha} = \sum_{\rho=1} \frac{\nu_{\rho\alpha} M_{\alpha}}{\rho} \dot{\zeta}_{\rho}$, $\dot{\zeta}_{\rho} = \frac{\dot{n}_{\rho}}{\nu_{\rho}} = \frac{\rho \dot{w}_{\rho}}{\nu_{\rho} M_{\rho}}$

Stress tensor $\mathbf{t} = \sum_{\alpha} (\mathbf{t}_{\alpha,el} + \mathbf{t}_{\alpha,dis})$ is split in elastic and dissipative parts.

Balance of entropy – II. Law of Thermodynamics

Entropy balance-general concept

All actual cyclical processes $\mathcal{C}$ running in the system $\mathcal{V}$ during which it is possible to measure the temperature T at any moment, must to fulfil the inequality

$$\oint \frac{dQ}{T} = \int_{t_1}^{t_2} \frac{\dot{Q}}{T} dt \leq 0 \quad \text{Clausius inequality}$$

i.e., some amount of heat has to be removed from the system

Entropy is defined by the inequality

$$TdS = TdS_{\text{ir}} + TdS_{\text{eq}} \geq dQ \quad \text{for} \quad TdS_{\text{eq}} = dQ$$

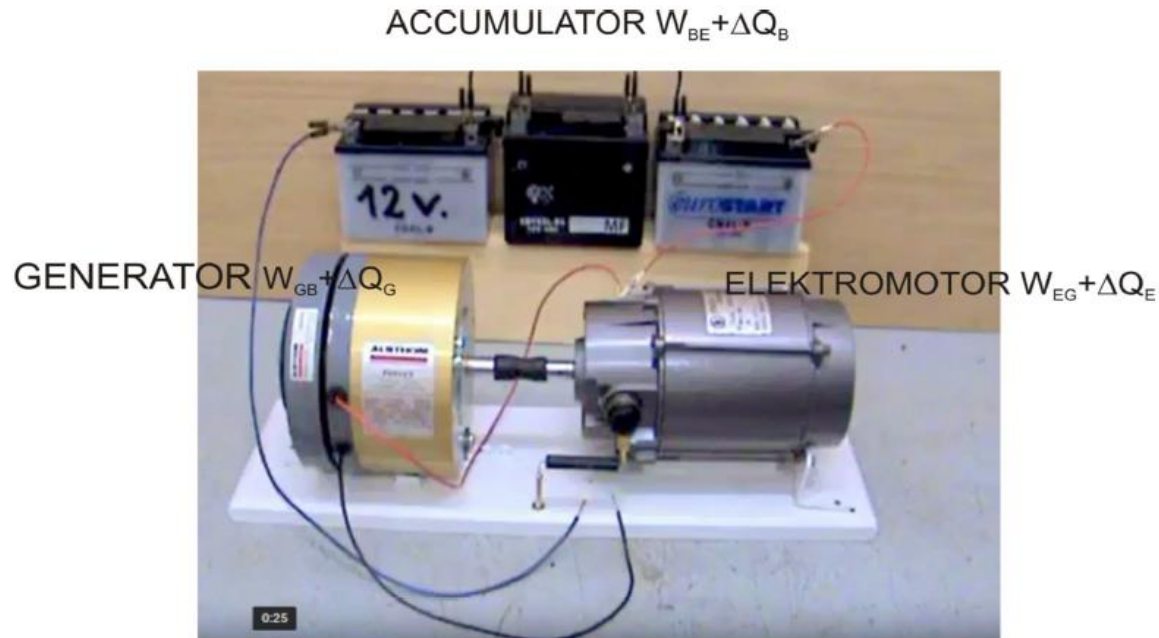
$$T\dot{S} = T\dot{S}_{\text{ir}} + T\dot{S}_{\text{eq}} \geq \dot{Q} \quad \text{for} \quad T\dot{S}_{\text{eq}} = \dot{Q}$$

$$\dot{S} - \mathcal{J}(S) = \mathcal{P}(S) \geq 0 \quad \text{II. Law of Thermodynamics}$$

$$\text{for } S = \int_{\mathcal{V}} \rho s d\nu, \quad \mathcal{J}(S) = \int_{\partial\mathcal{V}} -\frac{q}{T} da + \frac{q^{\text{ex}}}{T} d\nu,$$

$$\mathcal{P}(S) = \int_{\mathcal{V}} \sigma(S) d\nu \geq 0 \quad \text{entropy production is always positive}$$

Cyclic process



I. Law of Thermodynamics - Balance of total energy

$$W_{BE} + W_{EG} + W_{GB} + \Delta Q_B + \Delta Q_E + \Delta Q_G = \text{Total Energy is const.}$$

For $\Delta Q_B < 0, \Delta Q_E < 0, \Delta Q_G < 0 \dots$ is removed

II. Law of Thermodynamics - Process Irreversibility

$$W_{BE} > W_{GB}$$

Entropy definition

$$\begin{aligned} \dot{S} - \mathcal{J}(S) &= \mathcal{P}(S) \geq 0 \quad \text{II. Law of Thermodynamics} \\ \text{for } S &= \int_{\mathcal{V}} \rho s d\nu, \quad \mathcal{J}(S) = \int_{\partial\mathcal{V}} -\frac{q}{T} da + \int_{\mathcal{V}} \frac{q^{\text{ex}}}{T} d\nu, \\ \mathcal{P}(S) &= \int_{\mathcal{V}} \sigma(S) d\nu \geq 0 \end{aligned}$$

By eliminating the external heat source q^{ex} using the I. Law of Thermodynamics (Balance of total energy), we get

$$\begin{aligned} \sigma(S) &= \underbrace{\rho \left[\dot{s} - \frac{\dot{u}}{T} - \frac{p}{T} \overline{\left(\frac{1}{\rho} \right)} \right]}_{=0 \Leftrightarrow \text{Gibbs definition of entropy} \cdots s = s(u, \rho)} \\ &+ q^k \frac{\partial}{\partial x^k} \left(\frac{1}{T} \right) + \frac{t_{dis}^{ki}}{T} \frac{\partial v^i}{\partial x^k} \geq 0 \end{aligned}$$

Gibbs definition of entropy

$$T\dot{s} = \dot{u} - \frac{\mathbf{t}_{el}}{\rho} : \mathbf{d} - \sum_{\alpha} \mu_{\alpha} \dot{w}_{\alpha} \quad \text{for solids}$$

$$T\dot{s} = \dot{u} + p\left(\frac{\dot{1}}{\rho}\right) - \sum_{\alpha} \mu_{\alpha} \dot{w}_{\alpha} \quad \text{for fluids}$$

Chemical potential is defined as

$$\mu_{\alpha}(T, p, w_{\alpha}) = \bar{\mu}_{\alpha}(T, p) + \frac{RT}{M_{\alpha}} \ln x_{\alpha} \left[\frac{\text{J}}{\text{kg}} \right], \quad \text{for } x_{\alpha} = \frac{n_{\alpha}}{n} = \frac{w_{\alpha}}{M_{\alpha} \sum_{\beta} \frac{w_{\beta}}{M_{\beta}}}$$

Balance of entropy based on Gibbs definition

$$J_D(S) = - \int_{\partial\mathcal{V}} \frac{\mathbf{j}_q}{T} \mathbf{d}\mathbf{a} + \int_{\mathcal{V}} \frac{Q^{ext}}{T} d\nu, \quad \text{for one component system}$$

$$\begin{aligned} J_D(S) &= - \int_{\partial\mathcal{V}} \mathbf{j}(s) \mathbf{d}\mathbf{a} = - \int_{\partial\mathcal{V}} \left(\sum_{\alpha} \mathbf{j}_{D\alpha} s_{\alpha} + \frac{\mathbf{j}_q}{T} \right) \mathbf{d}\mathbf{a} \\ &= - \int_{\partial\mathcal{V}} \frac{\mathbf{j}_q}{T} \mathbf{d}\mathbf{a} - \int_{\partial\mathcal{V}} \frac{\sum \mathbf{j}_{D\alpha} h_{\alpha}}{T} \mathbf{d}\mathbf{a} + \int_{\partial\mathcal{V}} \frac{\sum \mathbf{j}_{D\alpha} \mu_{\alpha}}{T} \mathbf{d}\mathbf{a} \\ &= J_q(S) + J_{Dh}(S) - J_{Dg}(S) \quad \text{for multi-component system} \end{aligned}$$

and entropy production in the volume $\mathcal{V}$

$$P(S) = \int_{\mathcal{V}} \sigma(s) d\nu = \int_{\mathcal{V}} \sum_{\beta} J_{\beta}(X_{\gamma}) X_{\beta} d\nu \geq 0$$

$$\text{close to equilib. } J_{\beta} = \sum_{\gamma} \frac{\partial J_{\beta}}{\partial X_{\gamma}} X_{\gamma} + O(X_{\gamma}) = \sum_{\beta, \gamma} L_{\beta, \gamma} X_{\gamma}, \quad \beta, \gamma = 1, 2, \dots$$

$$\sigma(s) = \sum_{\beta} J_{\beta} X_{\beta} = \sum_{\beta, \gamma} L_{\beta, \gamma} X_{\beta} X_{\gamma}, \quad \beta, \gamma = 1, 2, \dots$$

$$\text{Density of entropy production } \sigma(S) = \sum_{\gamma} J_{\gamma} X_{\gamma} = \sum_{\beta, \gamma} L_{\beta\gamma} X_{\beta} X_{\gamma} \geq 0$$

$$T\sigma(S) = -\frac{\mathbf{j}_q}{T} \nabla T + \mathbf{t}_{dis} \mathbf{d} + \mathbf{j}_e \mathbf{E} \geq 0, \quad \text{for one component system} \quad (2.9)$$

$$\begin{aligned} \sigma(S) = & \left[\mathbf{j}_q + \sum \mathbf{j}_{D\alpha} h_{\alpha} + \mathbf{v}_{D\alpha} \cdot \mathbf{t}_{dis\alpha} \right] \cdot \nabla \left(\frac{1}{T} \right) + \frac{1}{T} \left[\mathbf{t}_{dis} - \sum_{\alpha} \rho_{\alpha} \mathbf{v}_{D\alpha} \otimes \mathbf{v}_{D\alpha} \right] : \mathbf{d} \\ & - \sum \mathbf{j}_{D\alpha} \cdot \left[\nabla \left(\frac{\mu_{\alpha}}{T} \right) - \frac{\mathbf{b}_{\alpha}}{T} - \frac{\mathbf{\Gamma}_c}{T} \right] + \sum_{\rho} \frac{\mathcal{A}_{\rho} \dot{\zeta}_{\rho}}{T} \geq 0 \end{aligned} \quad (2.10)$$

From the structure of the density of entropy production $\sigma(S)$ follows the dependence of the thermodynamic fluxes J_{β} on the thermodynamic forces X_{γ} . This is the intended result of classical nonequilibrium thermodynamics [4],[5].

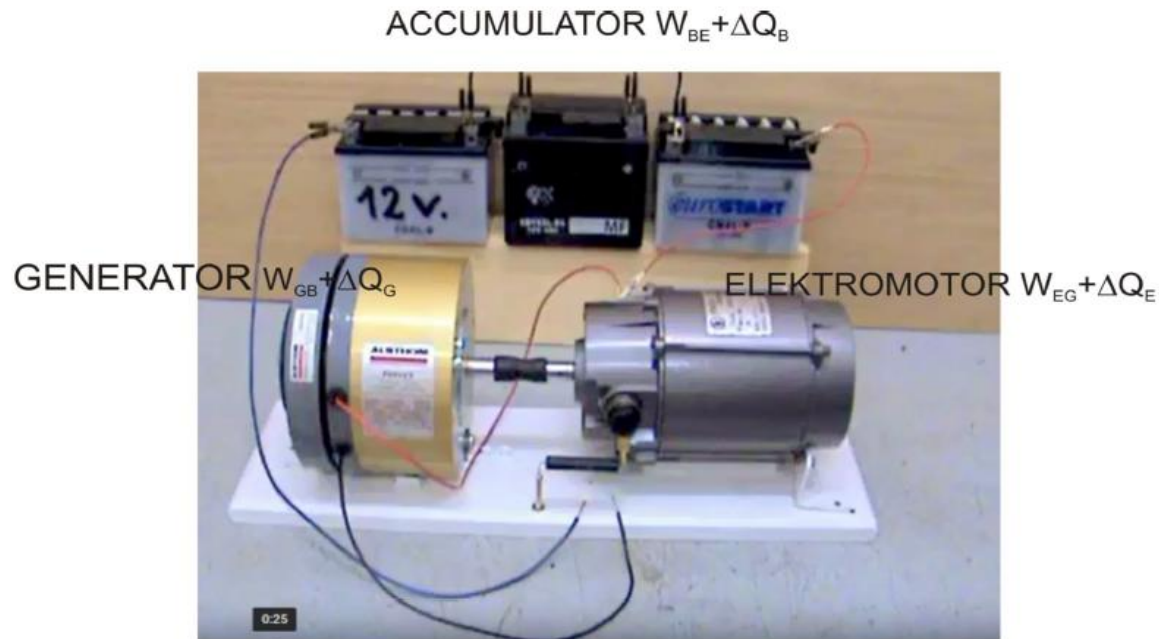
Entropy production for chemically reacting mixture

Typical form of transport processes $\mathbf{J}$ and their driving forces $\mathbf{X}$ in the thermodynamic systems (chemical devices). Corresponding entropy production is

$$\begin{aligned}\mathcal{P}(S) &= \sum_{\alpha} \mathbf{J}_{\alpha} \mathbf{X}_{\alpha} \geq 0 \\ &= \underbrace{\mathcal{P}(S_0)}_{\geq 0} + \underbrace{\delta \mathcal{P}(S_0)}_{=0} + \underbrace{\delta^2 \mathcal{P}(S_0)}_{=\sum_{\alpha} \delta \mathbf{J}_{\alpha} \delta \mathbf{X}_{\alpha} = \frac{1}{2} \dot{d}^2 S_{eq} \geq 0} + \dots \geq 0\end{aligned}$$

	Flux $\mathbf{J}_{\alpha}$	Force $\mathbf{X}_{\alpha}$
heat flux	$\dot{\mathbf{j}}_q$	$\nabla \left(\frac{1}{T} \right)$ -heat release
thermodiffusion	$\dot{\mathbf{j}}_{D_{\alpha}} h_{\alpha}$	$\nabla \left(\frac{1}{T} \right)$ -fuel delivery
concentration diffusion	$\dot{\mathbf{j}}_{D_{\alpha}}$	$\left(\frac{\nabla \mu_{\alpha}}{T} \right)$ -water dif. in PEM
electric current	$\dot{\mathbf{j}}_{e, \alpha}$	$\frac{F_{\alpha}}{T} = -\frac{z_{\alpha} F}{M_{\alpha} T} \nabla \phi$ -proton flux
visco-plastic processes for solids	$\mathbf{t}_{dis} (T, \mathbf{d}, \dot{\mathbf{t}}_{dis})$	$\frac{\mathbf{d}}{T}$
viscosity	$\mathbf{t}_{dis} - \sum_{\alpha} \rho_{\alpha} \mathbf{v}_{D_{\alpha}} \otimes \mathbf{v}_{D_{\alpha}}$	$\frac{(\sigma)}{T}$
swelling	$\mathbf{t}_{dis} \cdot \nabla \left(\frac{1}{T} \right)$	$\mathbf{v}_{D_{\alpha}}$
capillary flux	$\dot{\mathbf{j}}_{D_c}$	$\frac{\mathbf{r}_c}{T} = +\frac{1}{T} \nabla (\sigma \cdot \mathbf{a})$
chemical reaction and phase transition	$\dot{\xi}_{\rho}$	$\frac{A_{\rho}}{T}$ - at CL and GDL

Cyclic process



I. Law of Thermodynamics - Balance of total energy

$$W_{BE} + W_{EG} + W_{GB} + \Delta Q_B + \Delta Q_E + \Delta Q_G = \text{Total Energy is const.}$$

For $\Delta Q_B < 0, \Delta Q_E < 0, \Delta Q_G < 0$... is removed

II. Law of Thermodynamics - Process Irreversibility

$$W_{BE} > W_{GB}$$

Perpetuum mobile

I. type – violation of the law of total energy balance

$$\int dQ - \int dU - \int dW = 0$$

II. type – lossless transformation of individual types of energy
between each other

$$\int TdS - \int dU - \int dW = P(S) \geq 0$$

$$dQ = - \int_{\partial \mathcal{V}} \mathbf{q} \, \mathbf{da} = TdS - P(S) \Leftrightarrow \text{heat supplied across the system boundary } \partial \mathcal{V}$$

$$dQ \leq TdS, \quad P(S) \Leftrightarrow \text{heat generated during energy transformation}$$

Atomic structure

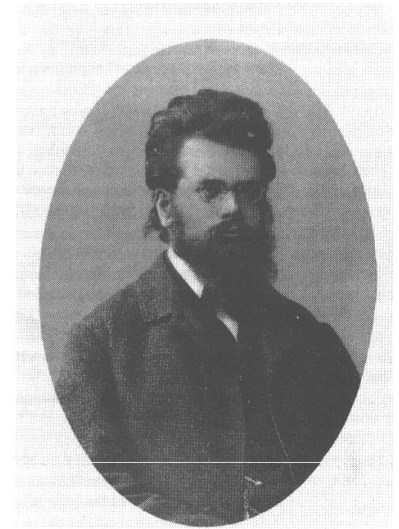
Ludwig Boltzmann (1844 -1906)

Statistical thermodynamics

$$S = k \ln Pr$$

Boltzmann equation for molecular collisions

Maxwell-Boltzmann distribution



Bring vor, was wahr ist;
Schreib' so, daß klar ist
Und verficht's, bis es mit dir gar ist

Say what is true;
Write it so that it is clear
And defend it until you are satisfied

ENTROPY S

(Greek origin $\epsilon\nu\tau\rho\omicron\pi\iota\alpha$ - change inside) - macroscopic quantity exhibiting collective properties of matter; a measure of randomness in an evolution of a system

R. Clausius - **1865**; $dS \geq \frac{dQ}{T}$ - **phenomenological approach**

L. Boltzmann - **1877**; $S = -k \int F \ln F d\mathbf{v}$ - **microscopical approach**

*** J. W. Gibbs** - **1900**; $S = k \ln \Gamma$ - **probabilistic approach**

A. Einstein - **1910**; $d^2S < 0$ - **thermodynamics of fluctuations**

Fluctuations around the equilibrium (reference) state reduce the entropy of the system.

*** L. Onsager** - **1933**; $P(S) = \sum J_i X_i > 0$
 $J_i = L_{ij} X_j$ - **cross effect**

E. Schrödinger - **1945**; - **each biological system is driven by a flux of negative entropy**

I. Prigogine - **1947**; $\frac{dP(S)}{dt} \geq 0$ - **principle of minimum entropy production**

*** M. Eigen** - **1957**; $\min P(S)$ - **competition between polymers**

All proteins on Earth are made up of only 20 amino acids

*** I. Prigogine** - **1977**; - **theory of open systems**

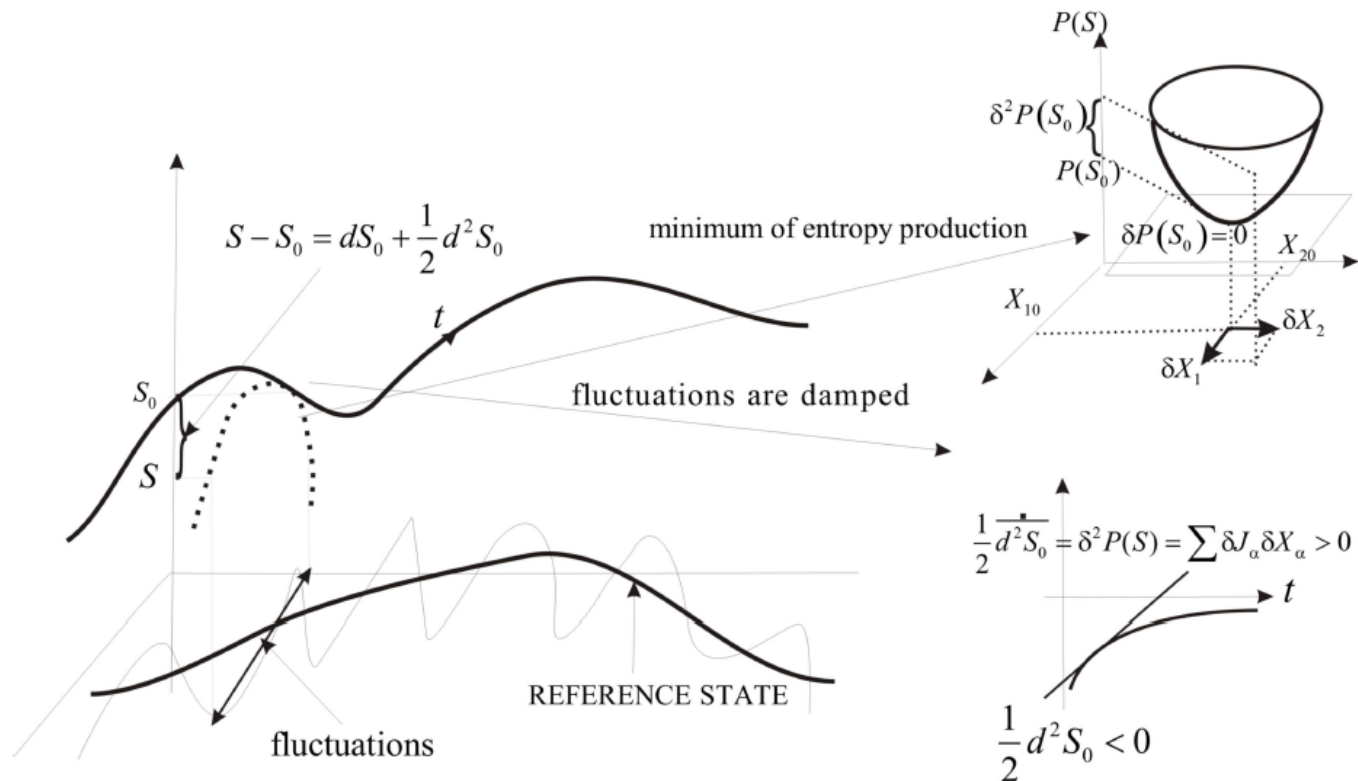
The stability of an open system is ensured by its growth.

Entropy production and damping of fluctuations

The entropy is convex function of its parameters, which fluctuates around the stable reference state S_0 , which can be even the non-equilibrium state. For the purely equilibrium state S_{eq} the fluctuations disappear. In the reference state the entropy has local maximum, i.e., $dS|_0 = 0$.

The probability of fluctuations is

$$\text{Pr} = \frac{\Gamma_{\text{noneq}}}{\Gamma_{\text{eq}}} = \exp \left[\frac{S - S_0}{k} \right] = \exp \left[\frac{d^2 S_0}{2k} \right] \dots \text{Einstein 1910}$$



Normal (Gaussian) distribution of fluctuations

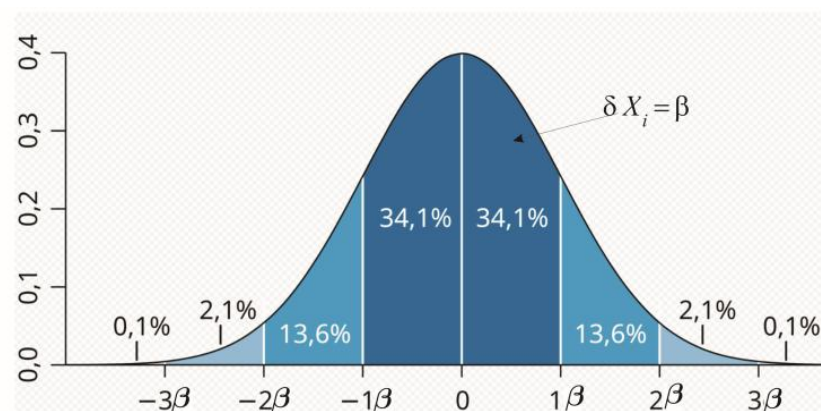
If we assume that the system contains a sufficient number of particles, and is close to a stable dynamic equilibrium, then we can only consider a normal (Gaussian) distribution. We will start from the relation for the probability distribution of acting quantities X_i around the reference (or equilibrium) X_{i0}

$$f(X_i|X_{i0}, \beta_i) = \frac{1}{\sqrt{2\pi\beta_i^2}} \exp \left[-\frac{(X_i - X_{i0})^2}{2\beta_i^2} \right] \sim \exp \left(\frac{d^2s}{2R} \right) \quad (3.1)$$

$$\text{Var}(X_i) = \langle X_i^2 \rangle - \langle X_i \rangle^2 = \beta_i^2 = (\delta X_i)^2,$$

$$\text{for } \langle X_i^2 \rangle = \int_{-\infty}^{\infty} X_i^2 f(X_i|X_{i0}, \beta_i) dX_i, \quad \langle X_i \rangle = X_{i0}$$

For the sake of clarity, we denote the variance $\text{Var}(X_i)$ of the quantity X_i as $(\delta X_i)^2 = \beta_i^2$. *Variance* is often called dispersion or standard deviation. From now on, we will use the term *dispersion* for this quantity.



Expansion near the equilibrium (reference) state

$$\dot{S} - \underbrace{\mathcal{J}(S)}_{\text{interaction with surroundings}} = \underbrace{\mathcal{P}(S)}_{\text{production inside}} \geq 0 \quad \text{Balance of entropy}$$

The balance of entropy closed to the reference state is

$$\text{Entropy} \cdots S = S_0 + \underbrace{\delta S_0}_{\text{shift of the reference state}} + \underbrace{\frac{1}{2}\delta^2 S_0}_{\leq 0 \text{ fluctuations inside the system}} + \cdots$$

$$\text{Entropy flux} \cdots \mathcal{J}(S) = \mathcal{J}(S_0) + \underbrace{\delta \mathcal{J}(S_0)}_{\text{change of external fluxes}} + \underbrace{\frac{1}{2}\delta^2 \mathcal{J}(S_0)}_{\text{change of internal fluxes}} + \cdots$$

$$\text{Entropy production} \cdots \mathcal{P}(S) = \mathcal{P}(S_0) + \underbrace{\delta \mathcal{P}(S_0)}_{=0 \text{ minimum}} + \underbrace{\frac{1}{2}\delta^2 \mathcal{P}(S_0)}_{\geq 0 \text{ excess of entropy}} + \cdots$$

Finally

$$\begin{aligned} & \underbrace{\dot{S}_{\text{eq}} - \mathcal{J}(S_{\text{eq}})}_{=0, \mathcal{P}(S_{\text{eq}})=0} + \underbrace{\overline{\delta \dot{S}_0} - \delta \mathcal{J}(S_0)}_{\text{the shift of a reference state}} \\ & - \underbrace{\mathcal{P}(S_0)}_{\geq 0} + \underbrace{\frac{1}{2}\overline{\delta^2 \dot{S}_0} - \frac{1}{2}\delta^2 \mathcal{J}(S_0) - \delta \mathcal{P}(S_0) - \frac{1}{2}\delta^2 \mathcal{P}(S_0)}_{\rightarrow 0 \text{ non-equilibrium processes inside}} = 0 \end{aligned}$$

Thermodynamic stability condition

The reference (equilibrium) state is defined as

$$\dot{S}_{\text{eq}} = J(S_{\text{eq}}), \quad \text{when} \quad \mathcal{P}(S_{\text{eq}}) = 0 \quad \text{for equilibrium reference state } S_{\text{eq}}$$

$$\dot{\overline{S}}_0 - \delta \mathcal{J}(S_0) = \mathcal{P}(S_0) \geq 0 \quad \text{for non-equilibrium reference state } S_0$$

The reference state S_0 is stable under the following conditions

$$\frac{1}{2} \dot{\overline{S}}_0 = \underbrace{\frac{1}{2} \delta^2 \mathcal{P}(S)}_{=\sum_{\alpha} \delta J_{\alpha} \delta X_{\alpha} \geq 0} + \underbrace{\delta \mathcal{P}(S_0)}_{\rightarrow 0 \text{ extremum (minimum)}} + \underbrace{\frac{1}{2} \delta^2 \mathcal{J}(S_0)}_{\rightarrow 0 \text{ internal fluxes}}$$

which are satisfied inside the system. Their meaning is

- ▶ Minimum of entropy production

$$\delta \mathcal{P}(S_0) = 0, \quad \delta^2 \mathcal{P}(S_0) > 0$$

- ▶ Additional condition for internal entropy flux

$$\delta^2 \mathcal{J}(S_0) \neq 0 \quad \text{entropy flux is}$$

compensated by fluctuations on the boundary

$$\delta^2 \mathcal{J}(S_0) = 0 \quad \text{entropy flux is fixed;}$$

so called **condition of endoreversibility**

- ▶ Attenuation of the fluctuations

$$\frac{1}{2} \dot{\overline{S}}_0 = \sum \delta J_{\alpha} \delta X_{\alpha} \geq 0$$

Standard deviation or dispersion (often called variance) of fluctuations for Gibbs entropy $Tds = du + pd\left(\frac{1}{\rho}\right) - \sum_{\alpha} \mu_{\alpha} dw_{\alpha}$

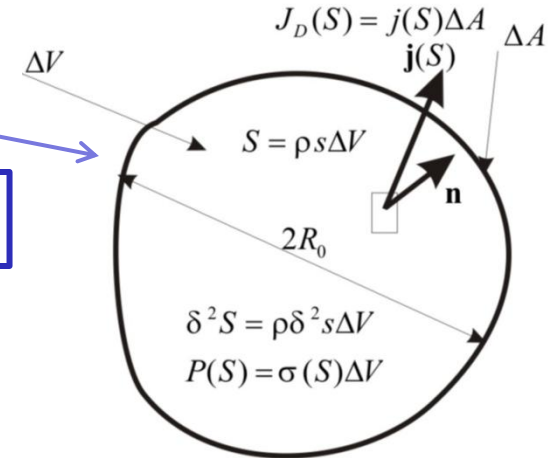
We will adjust the second differential of entropy (3.2) to a form suitable for some small element of the ΔV system, see Fig. 3.2

$$\delta^2 S = \rho \delta^2 s \Delta V = -\rho \Delta V \left(a_T (\delta T)^2 + a_{\rho} (\delta(1/\rho))_{w_{\alpha}}^2 + \sum_{\alpha} a_{\alpha} (\delta n_{\alpha})^2 \right)$$

$$= -\rho \Delta V \left[\frac{c_v}{T^2} (\delta T)^2 + \frac{\rho}{\chi} (\delta(1/\rho))_{w_{\alpha}}^2 + \frac{1}{\rho T} \sum_{\alpha=1}^r \left(\frac{\partial \mu_{\alpha}}{\partial n_{\alpha}} \right)_{T,p} (\delta n_{\alpha})^2 \right] < 0$$

$$\text{for } \mu(p, T, n_{\alpha}) = \frac{RT}{M_{\alpha}} \ln \left(\frac{n_{\alpha}}{n_{tot}} \right), \quad w_{\alpha} = \frac{M_{\alpha} n_{\alpha}}{\rho}, \quad n_{tot} = \sum_{\alpha=1}^r n_{\alpha}$$

The coefficient $a_T, a_{\rho}, a_{\alpha}$ are defined by this relation. We will now assume that the fluctuations of temperature, density and concentration are independent of each other.



Dispersion of temperature

$$\frac{\overline{(\delta T)^2}}{T^2} = \frac{nR}{\rho c_v} \left(= \frac{R}{c_{v\alpha} M_{\alpha}} \right), \quad c_v = \sum_{\alpha} w_{\alpha} c_{v\alpha} > 0$$

thermal stability condition

Dispersion of density

$$\rho^2 \overline{\left(\delta \left(\frac{1}{\rho} \right)_{w_{\alpha}} \right)^2} = \frac{nRT}{\rho c_T^2}, \quad (=1) \quad c_T^2 = \hat{R}T > 0$$

mechanical stability condition.

In a one-component gas, the dispersion of fluctuations of the specific volume $v = 1/\rho$ is equal to the square of the density ρ^2 . Also interesting is the fluctuation of concentration

$$\sum_{\alpha, \alpha'=1}^r \left(\frac{\partial \mu_{\alpha}}{\partial w_{\alpha'}} \right)_{T,p,w_{\alpha''}} \delta w_{\alpha} \delta w_{\alpha'} > 0 \quad \text{stability condition of diffusion}$$

which for the α component is equal to its actual concentration

Dispersion of concentration

$$\overline{(\delta w_{\alpha})^2} = \frac{nRT}{\rho} \left(\frac{\partial \mu_{\alpha}}{\partial w_{\alpha}} \right)_{T,p,w_{\alpha'}}^{-1} \left(= \frac{nM_{\alpha}}{\rho} w_{\alpha} \right) > 0$$

Properties of fluctuations in the thermodynamic steady state

The reference state S_0 is stable under the following conditions

$$\overline{\delta^2 \dot{S}_0} - \delta^2 \mathcal{P}(S) - 2\delta \mathcal{P}(S_0) - \delta^2 \mathcal{J}_D(S_0) \rightarrow 0$$

We will limit ourselves to diffusion and chemical reaction only.

$$\rho a_\alpha \overline{(\delta n_\alpha)^2} + \sigma_\alpha (\delta n_\alpha)^2 = -\delta^2 j_\alpha(S_0) \left(\frac{\Delta A}{\Delta V} \right)$$

$\frac{2}{R_0}$

$$(\delta n_\alpha)^2(t) + \frac{2\delta^2 j_\alpha(S_0)}{\sigma_\alpha R_0} = \left[(\delta n_\alpha)_0^2 + \frac{2\delta^2 j_\alpha(S_0)}{\sigma_\alpha R_0} \right] \exp \left[-\frac{\sigma_\alpha}{\rho a_\alpha} (t - t_0) \right]$$

for $(\delta n_\alpha(t = t_0))^2 = (\delta n_\alpha)_0^2$

Since term $\sigma_\alpha/(\rho a_\alpha)$ is related to dissipation⁵ and is always positive, the right-hand side of the equation goes to zero and the magnitude of the fluctuation dispersion is equal to

$$(\delta n_\alpha)^2(t) \stackrel{t \gg t_0}{\rightarrow} -\frac{2\delta^2 j_\alpha(S_0)}{\sigma_\alpha R_0} > 0$$

where $\delta^2 \mathbf{j}_\alpha(S_0) \mathbf{n} = -\delta^2 j_\alpha(S_0) = -\frac{v_{D_\alpha} R}{n_\alpha} (\delta n_\alpha)_0^2$ flux in the ΔV .

Condition of steady state stability

$$\frac{(\delta n_\alpha)^2}{(\delta n_\alpha)_0^2} \geq_{t \gg t_0} \frac{2j_{D_\alpha}(S_0)}{\Sigma_\alpha(S) R_0}$$

Comparison with thermodynamic uncertainty relation (TUR)

It has been found that in steady state the ratio of dispersion (variance) to mean can be universally bounded by the entropy production:

The greater the entropy production $\Sigma(S)$, the less the quantity J_τ fluctuates around the equilibrium (reference) value.

$$\frac{\text{Var}(J_\tau)}{\langle J_\tau \rangle^2} = \frac{(\delta J_\tau)^2}{\langle J_\tau \rangle^2} \geq \frac{2R}{\Sigma(S)\tau} \quad \text{for } R - \text{Gas constant} \\ \tau \text{ -- observation time}$$

We modify the **stability condition** into a form similar to the relation describing **thermodynamic uncertainty** for the case of diffusion accompanied by chemical reaction

$$\frac{(\delta n_\alpha)^2}{n_{\alpha 0} n_{tot}} \geq_{t \gg t_0} \frac{2j_{D_\alpha}(S_0)}{\Sigma_\alpha(S_0)R_0} \quad \text{for } R_0 \text{ -- geometric size} \\ \text{of the area}$$

The greater the entropy production, the less the concentration fluctuates around the equilibrium (reference) value..

Comparison with quantum mechanical uncertainty:

$$\Delta E \Delta t \geq \frac{h}{2\pi}$$

The faster the **particle decay** (the shorter its **lifetime**), the less certain is its **mass** (the larger the particle's **width**).

I. Prigogine - 1970

Theory of open systems

Decay of dissipative structure $P(S) \rightarrow 0$

Formation of a new dissipative structure
(by instability) $P(S) > 0$



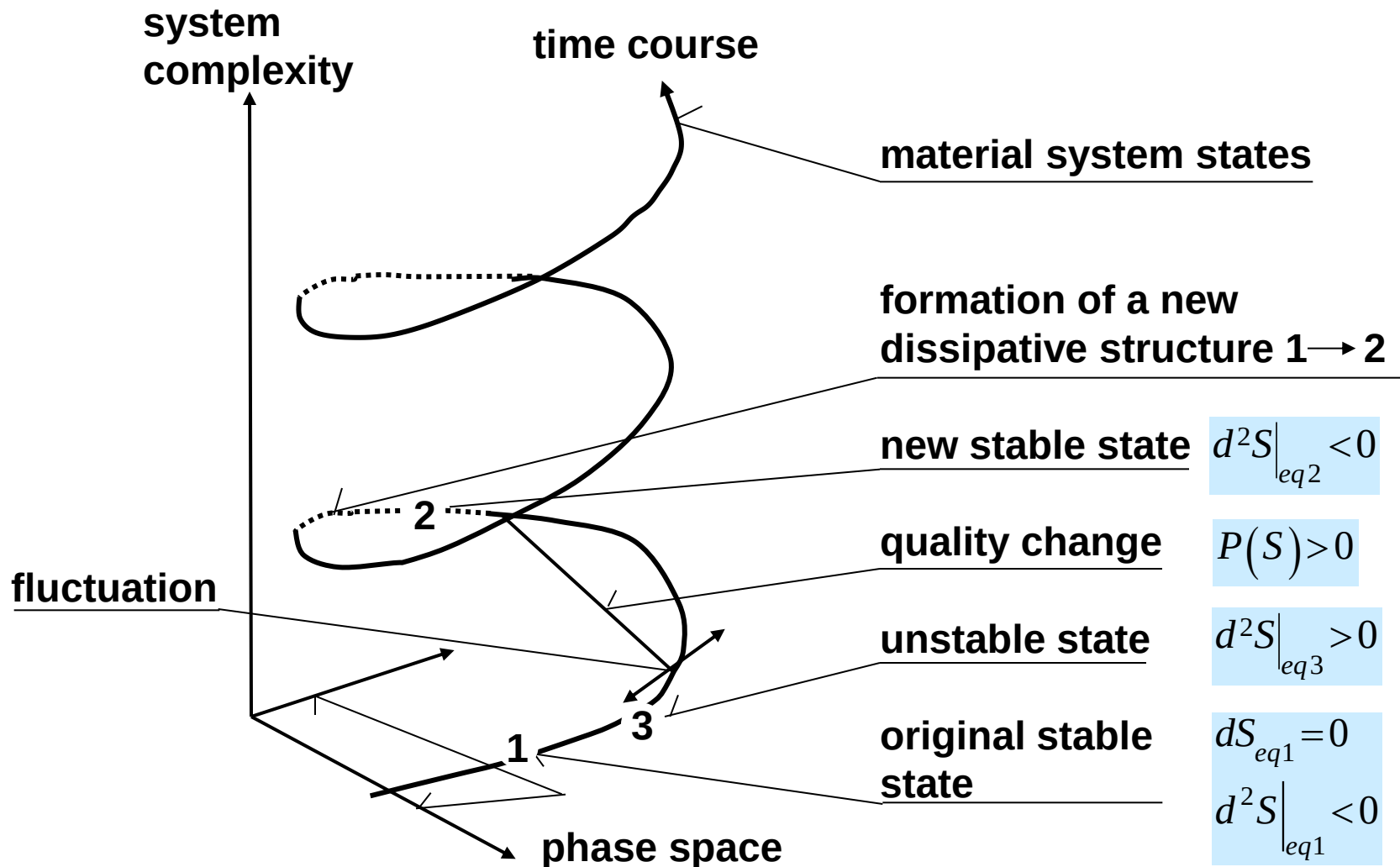
Path to equilibrium
-biological death



Path to a greater complexity and to a closer
interaction with surroundings

$$-J(S) = P(S) > 0$$

Thermodynamic view of the biological system evolution



Prof. Illya Prigogine receives the Nobel Price for Chemistry from the hands of Carl Gustav-the King of Sveden.



**Application of thermodynamic criteria
to systems with convection.**

Balance of energy-I. Law of thermodynamics and Balance of entropy-II. Law of thermodynamics

The **I. Law of Thermodynamic** formulated with the total enthalpy is given by

$$\rho \dot{h}_t - \frac{\partial p}{\partial t} = -\frac{q^k}{T} \frac{\partial T}{\partial x^k} + \frac{\partial(t_{dis}^{ki} v_i)}{\partial x^k} \quad \text{for} \quad h_t = \frac{v^2}{2} + u + \frac{p}{\rho} + \Phi$$

Definition of entropy S follows from the global form of the **II. Law of thermodynamics** formulated as the balance of the total entropy

$$\dot{S} - J_D(S) = P(S) \geq 0, \quad \text{for} \quad J_D(S) = - \int_{\partial V} \frac{q^i}{T} da_i, \quad P(S) = \int_V \sigma(s) d\nu \geq 0$$

where $J_D(S)$ is entropy flux, $P(S) \geq 0$ is total entropy production and $\sigma(S) \geq 0$ is the density of entropy production. Eliminating heat flux $\mathbf{q}$ by I. Law of thermodynamic we get II. Law of thermodynamic in the local form, so called **dissipative inequality**

$$\pi = T\sigma(S) = \underbrace{\rho \left(T\dot{s} + \frac{1}{\rho} \frac{\partial p}{\partial t} - \dot{h}_t \right)}_{=0 \dots \text{alternative definition of entropy}} - \frac{q^k}{T} \frac{\partial T}{\partial x^k} + \frac{\partial(t_{dis}^{ki} v_i)}{\partial x^k} \geq 0,$$

The thermodynamic stability criterion can be formulated by h_t . The entropy is the function of h_t, p and the thermodynamic inequality (II. Law of thermodynamics) is for $\pi < 0$ violated and the instability can occurs.

The same logical thinking was used
in deriving Gibbs' definition of entropy

$$\begin{aligned} \dot{S} - \mathcal{J}(S) &= \mathcal{P}(S) \geq 0 \quad \text{II. Law of Thermodynamics} \\ \text{for } S &= \int_{\mathcal{V}} \rho s d\nu, \quad \mathcal{J}(S) = \int_{\partial\mathcal{V}} -\frac{q}{T} da + \int_{\mathcal{V}} \frac{q^{\text{ex}}}{T} d\nu, \\ \mathcal{P}(S) &= \int_{\mathcal{V}} \sigma(S) d\nu \geq 0 \end{aligned}$$

By eliminating the external heat source q^{ex} using the I. Law of Thermodynamics (Balance of total energy), we get

$$\begin{aligned} \sigma(S) &= \underbrace{\rho \left[\dot{s} - \frac{\dot{u}}{T} - \frac{p}{T} \overline{\left(\frac{1}{\rho} \right)} \right]}_{= 0 \Leftrightarrow \text{Gibbs definition of entropy} \cdots s = s(u, \rho)} \\ &+ q^k \frac{\partial}{\partial x^k} \left(\frac{1}{T} \right) + \frac{t_{dis}^{ki}}{T} \frac{\partial v^i}{\partial x^k} \geq 0 \end{aligned}$$

Entropy for convection processes

The specific total enthalpy is a function of the entropy and the pressure, i.e. $h_t = h_t(s, p)$ and satisfies the general relation

$$\dot{h}_t = T\dot{s} + \frac{1}{\rho} \frac{\partial p}{\partial t}.$$

All dissipative processes in the system, which is in the thermodynamic equilibrium, which we will call a **reference state** (denoted by subscript "0"), are zero. Considering the rapid temporal change of fluctuations, this reference state changes only very slowly in time. For such a reference state, $h_{t0} = h_t(s_0, p_0)$ has a dissipation extremum, i.e. is equal to zero

$$T_0\dot{s}_0 - \dot{h}_{t0} + \frac{1}{\rho_0} \frac{\partial p_0}{\partial t} = 0, \quad \tilde{\pi} = \tilde{\pi}_0 = 0$$

Now, let us suppose that the system deviates ($s = s_0 + \delta s$, $p = p_0 + \delta p$) from this reference state and its total enthalpy changes. The deviations (fluctuations) δs , δp generate a dissipation $\tilde{\pi} \geq 0$, i.e.

$$T_0\dot{s} - \dot{h}_t + \frac{1}{\rho_0} \frac{\partial p}{\partial t} = \tilde{\pi}_0 + \tilde{\pi} = \tilde{\pi} \geq 0$$

Thermodynamic approach to fluid stability

For the simplified flow, $v_\varphi = v_\varphi(r)$, $T = T(r)$ has **thermodynamic condition of the stability** the form

$$\tilde{\pi} = \frac{\lambda}{T} \left(\frac{\partial T}{\partial r} \right)^2 + \mu \left[\left(\frac{\partial v_\varphi}{\partial r} \right)^2 + v_\varphi \frac{\partial^2 v_\varphi}{\partial r^2} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial r} \right] \geq 0 \quad (1)$$

Considering that the thermal conductivity $\lambda > 0$ and the viscosity $\mu > 0$ are positive coefficients and therefore the associated **blue terms** are always positive and will only have a stabilizing effect. We therefore focus only on the influence of the flow field shape $v_\varphi(r)$ and its derivatives, which plays a dominant role.

$$\begin{aligned} v_\varphi &= \omega r & \text{then } \tilde{\pi} &= 0 & \text{solid body vortex with angular velocity } \omega \\ v_\varphi &= \Gamma/r & \text{then } \tilde{\pi} &= 4\Gamma^2/r^4 \geq 0 & \text{potential vortex} \end{aligned} \quad (2)$$

The solid body vortex is on the onset of stability and the potential vortex with circulation Γ is stable.

To show the generality of the thermodynamic stability condition the following problems are studied:

- classical Taylor-Couette flow between two cylinders
- annular swirling jet transformation
- tropical cyclones-Rankine vortex approximation

Every vortex transforms into a potential vortex

Vortex tube transformation $\mathbf{v}_{\text{rot}} \longrightarrow \mathbf{v}_{\text{pot}}$

Thermodynamic stability condition

$$h_t = u + \frac{p}{\rho} + \frac{v^2}{2} + \phi$$

$$-\frac{\rho}{2} \frac{d}{dt} d^2 h_t = \tilde{\pi} \geq 0 \dots \text{thermodynamic}$$

stability condition

$$\tilde{\pi} = \mu_{\text{air}} \left[\left(\frac{\partial \mathbf{v}_\varphi}{\partial r} \right)^2 + \mathbf{v}_\varphi \frac{\partial^2 \mathbf{v}_\varphi}{\partial r^2} - \frac{\mathbf{v}_\varphi}{r} \frac{\partial \mathbf{v}_\varphi}{\partial r} \right] \geq 0$$

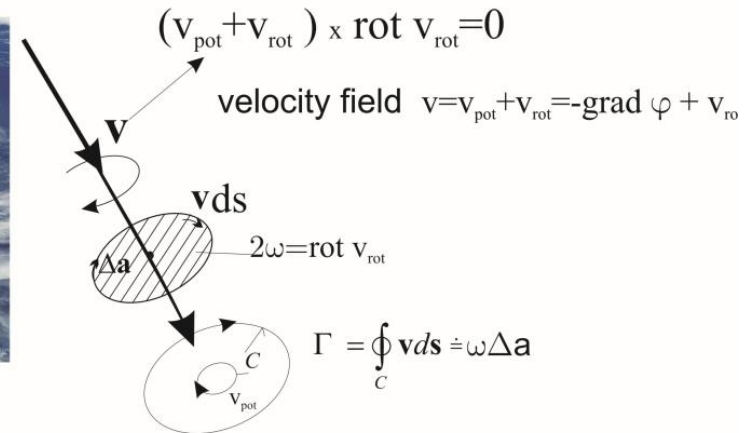
Stable

$$\mathbf{v}_\varphi(r) = \frac{\Gamma}{r} \Rightarrow \tilde{\pi} = \frac{4\Gamma^2}{r^4} > 0 \text{ potential vortex}$$

Unstable

$$\mathbf{v}_\varphi(r) = \omega r \Rightarrow \tilde{\pi} = 0 \text{ solid body vortex}$$

Tropical Cyclone Catarina from the International Space Station on March 26, 2004



A waterspout near the Florida Keys (15 miles south of Miami) Tornado over water



Balance laws

mass... $\text{div } \mathbf{v} = 0$

momentum... $\mathbf{v} \times \text{rot } \mathbf{v} = \text{grad } h_t - T \text{grad } s$

energy... $\dot{h}_t = 0$

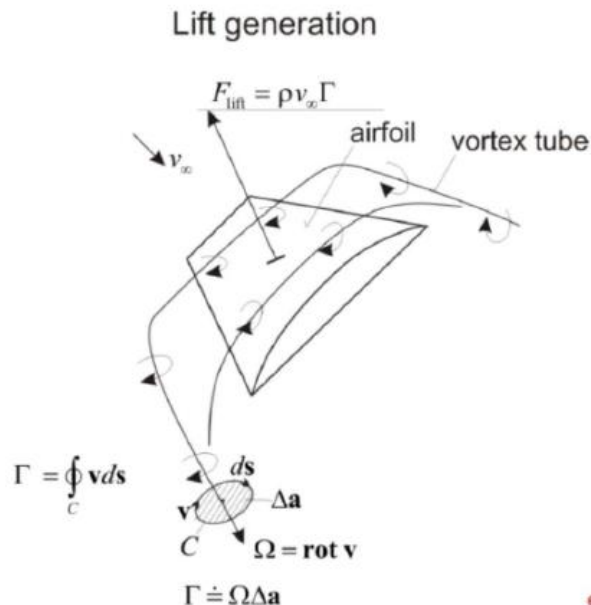
entropy... $T \text{grad } s = \text{condensation heat}$

Conclusion following from the energy balance formulated by the total enthalpy

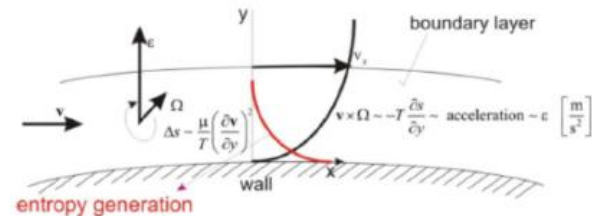
$$\Delta Q = \Delta H_c - \Delta_{ir} W_{mech}, \quad \Delta_t P = 0, \quad T \Delta S_{ir} = \text{viscous dissipation, phase transition heat, etc}$$

$$\Delta_{ir} W_{mech} = T \Delta S_{ir} \sim \mathbf{v} \times \mathbf{rot} \mathbf{v}, \quad \Gamma = \oint_C \mathbf{v} d\mathbf{s} = \oint_A \mathbf{rot} \mathbf{v} d\mathbf{a} \quad - \text{circulation}$$

Vortex Generation on body surface



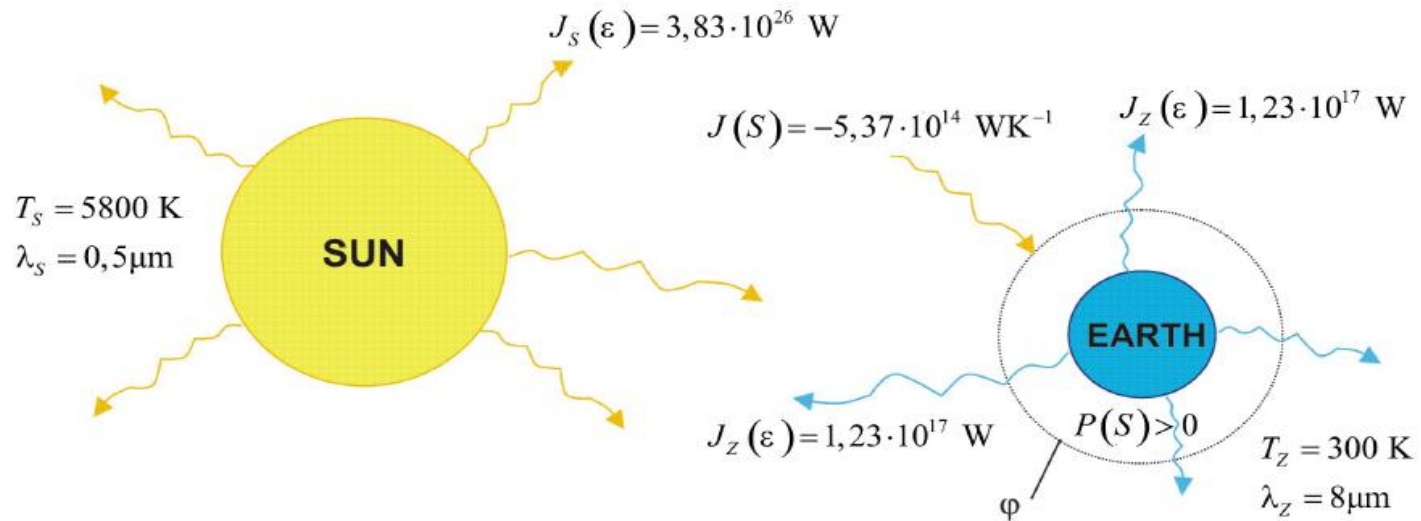
Vortex generation in boundary layer



Application to the Earth atmosphere:

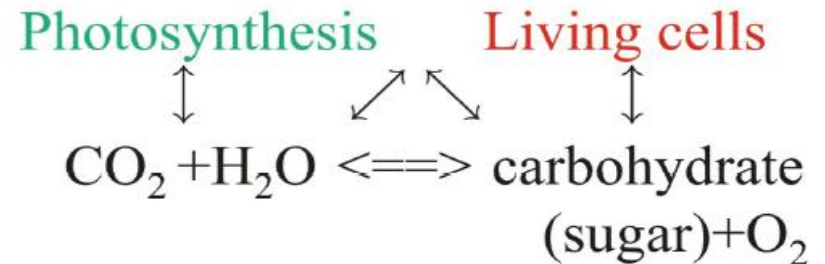
- Energy and entropy balance of the Earth
problem of warming
- Atmosphere instabilities
Tropical cyclones, Tornados (twisters)

ENTROPY BALANCE OF THE EARTH



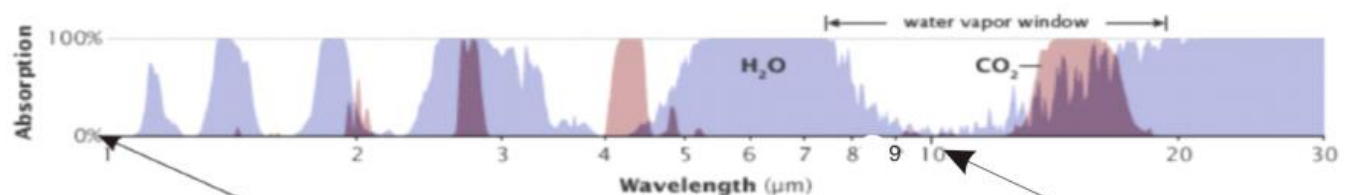
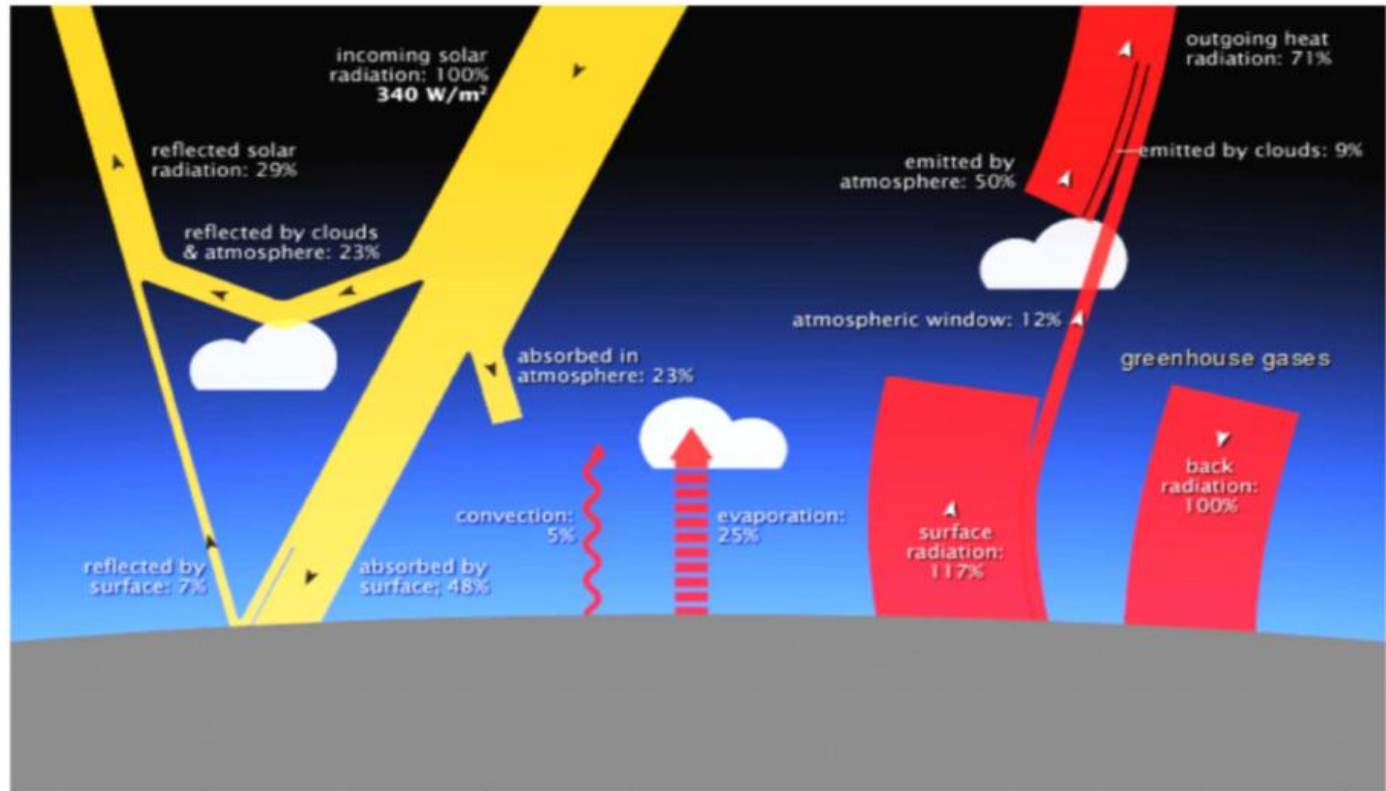
ENTROPY FLUX OF THE EARTH

$$J(S) = \frac{4}{3} \left(\frac{J_z(\epsilon)}{T_s} - \frac{J_z(\epsilon)}{T_z} \right) = -5,37 \cdot 10^{14} \text{ WK}^{-1}$$



Earth total energy income $5.46 \cdot 10^{24}$ J/year

29% of energy leaves the Earth in the form of radiation and 71% in the form of heat



Sun radiation $0.5 \mu\text{m}$

Earth radiation $10 \mu\text{m}$ at 17°C

Dynamical equilibrium assumption.

What is important is not the flow of energy, but the flow of negative entropy

$$-J(S) = P(S) = 5,37 \cdot 10^{14} \text{ W/K}$$

$$P_{rad}(S) = 0,94P(S) \text{ ...absorption and emission of energy}$$

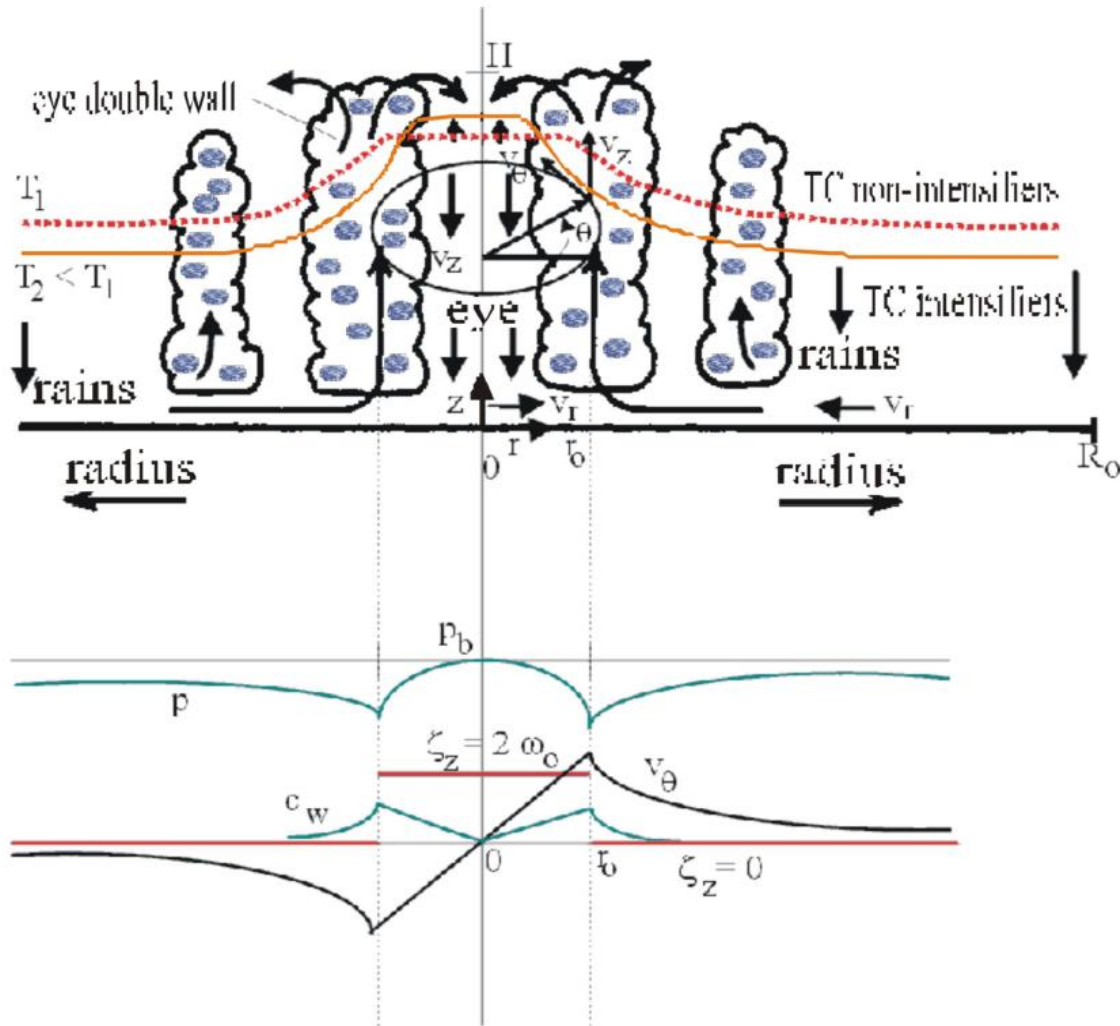
$$P_{transf}(S) = 0,06P(S) = 3,22 \cdot 10^{13} \text{ W/K...material changes on earth surface and movement of atmosphere}$$

Energy input from the Sun is 10^{17} W

Civilization generates power about 10^{13} W and corresponding entropy production is $P_{civ}(S) = 3 \times 10^{10} \text{ W/K} = 0,0008P_{transf}(S)$

The mere existence of 10 billion human beings in basal metabolism produces $P_{H.B.}(S) = 5 \times 10^9 \text{ W/K}$

Tropical cyclone structure



For a **tropical cyclone** of radius $r_o = 15$ km, the acceleration acting on the elements of air is

$$h_{vl} \frac{\partial c_w}{\partial r} = 4.2 \text{ m s}^{-2}$$

condensation heat of water vapor is $h_{vl} = 2.44 \text{ MJ/kg}$

For a **tornado** of radius $r_o = 50$ m, the acceleration acting on the elements of air is

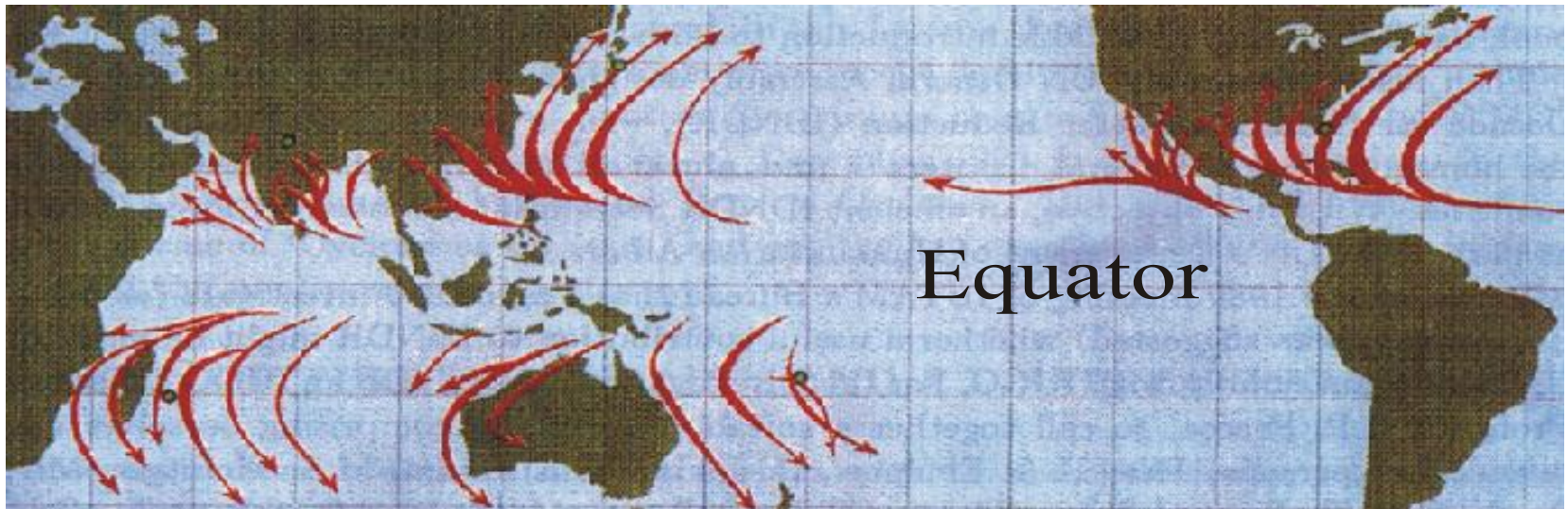
$$h_{vl} \frac{\partial c_w}{\partial r} = 65 g = 640 \text{ m s}^{-2}$$

3. Origination of tropical cyclones and tornadoes

The meaning of “**Cyclops**” in Greek is “ring-shaped eye” as well.

Three specific characteristics of the tropical cyclone (TC) are:

- a) an enormous dimension (often more than 2000 km),
- b) one ring-shaped eye (up to 30 km in size),
- c) extraordinary rage (the energy reaching up to 10^{18} J).

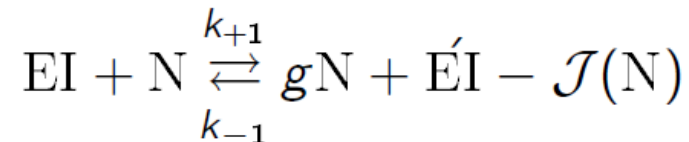


The most frequent routes of the tropical cyclones. Their average mean number on the Northern Hemisphere counts approximately 30, on the Southern hemisphere some ones less.

- **Application to living systems:**
- **Energetic limitations of population growth**
- **Dynamics of ecological system with migration**
- **Muscle contraction as a function of a molecular motor**
- **Basal metabolism in humans**

Energetic of population growth I

Population growth can be written as an analogy to auto catalysis in chemistry



where EI is surrounding interaction of individual N before reproduction and EI' is surrounding interaction of individual N after reproduction.

Rate of reproduction characterizes rate constant k_{+1} and rate of cessation characterizes rate constant k_{-1} . Migration flux is $\mathcal{J}(\text{N}) = \frac{N}{R}$. Here R is the resistance of the surroundings

- ▶ $g = 2$ proliferation-e.g., cells division
- ▶ $g \geq 3, 4, \dots$ number of descendants, e.g., sex reproduction.

Energetic of population growth II

Steady number of individuals is

$$N_0 = \frac{N_{EI}}{N'_{EI}} \exp \left[- \frac{\Delta G_N}{(g-1)RT} \right]$$

- ▶ $\Delta G_N < 0$... spontaneous process (without additional energy from surroundings); the material growth without energy is impossible
- ▶ $\Delta G_N > 0$...material growth needs some energy from outside

Competition between cell division (N_{0p} ...is number of individuals) and **sexual reproduction** (N_{0s} ... is number individuals) without migration.

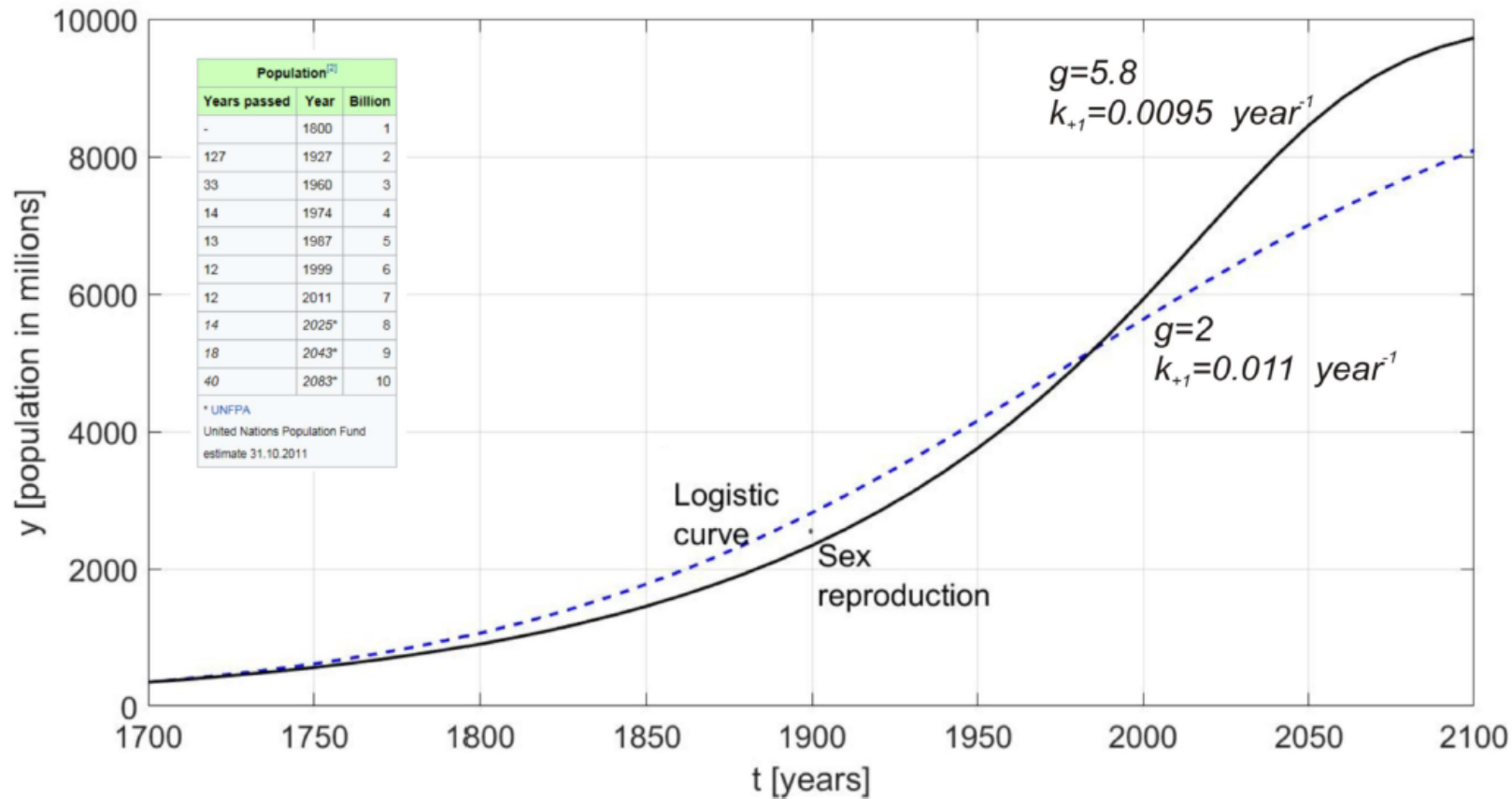
$$\frac{N_{0s}}{N_{0p}} = \exp \left[\frac{\Delta G_{Np}}{RT} \left(1 - \frac{\Delta G_{Ns}}{(g-1)\Delta G_{Np}} \right) \right] = 1, \quad \text{whence} \quad \Delta G_{Ns} = (g-1)\Delta G_{Np}$$

Sex reproduction is more expensive but more stable in variable environment. It has higher Gibbs free energy

- ▶ proliferation process (e.g., cell division) with $g = 2$. Division is fast, efficient with less energy expenditure (no mate searching), ideal for stable environments.
- ▶ sex reproduction with $g \geq 4$. Sexual reproduction produces genetic diversity that helps to survive in changing conditions and protect descendants from disease and parasites. The corresponding species is much more stable.

Human population

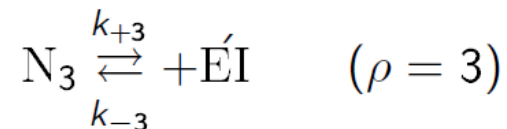
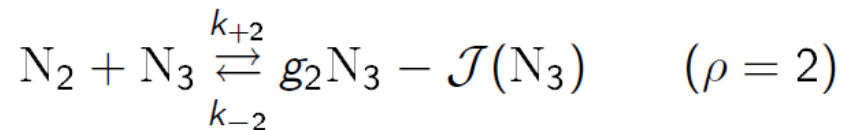
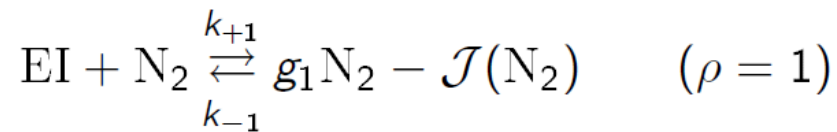
Two population models applied to evolution of the Earth.



Supposed stationary state is 10 billions. Sex reproduction curve is fitted to data from World population prospects.

Dynamics of predator N_3 -prey N_2 system: Lotka-Volterra model

Two competitive ecological systems (in general two auto catalytic reactions) of type predator N_3 and prey N_2 .

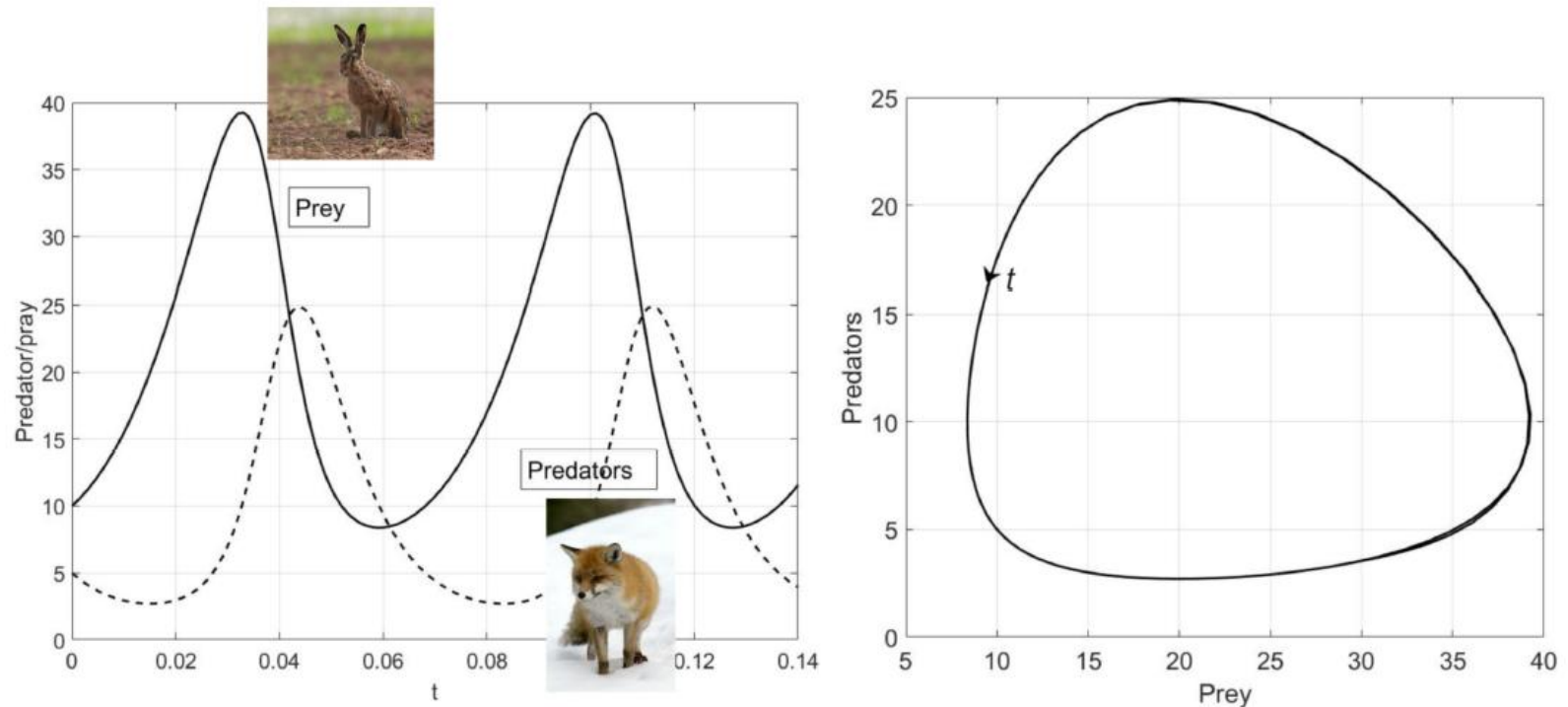


where EI is surrounding interaction before reproduction and $E'I$ is surrounding interaction after reproduction.

Rate of reproduction characterizes rate constant $k_{+\rho}$ and rate of cessation constant $k_{-\rho} \rightarrow 0$.

Parameter g complies condition $g_1, g_2 \geq 3, 4, \dots$ and depends on number of descendants. Migration fluxes are $\mathcal{J}(N_2)$ and $\mathcal{J}(N_3)$.

Dynamics of predator-prey competition: Lotka-Volterra model without migration



Dynamics of ecological model predators N_3 , preys N_2 , for stationary values $N_{30} = 10$, $N_{20} = 20$, with rate constant $k_{+1}N_{EI} = 70$, $k_{+2} = 7$ and time period $\tau = 0.064$.

Thermodynamically correct evolution is in direction of arrow because just evolution in this direction produces positive entropy.

Dynamics of predator-prey system: Lotka-Volterra model with migration

$$\omega = \omega_r + \omega_{im} = \omega_D \pm i\omega_D \sqrt{\left(\frac{\omega_0}{\omega_D}\right)^2 - 1}$$

$$\underbrace{\omega_D = \frac{(1+m)D_2k^2}{2}}_{\text{diffusion frequency for } D_3 = mD_2}, \quad \underbrace{\omega_0 = \sqrt{k_{+2}N_{20}N_{30}}}_{\text{predator-prey frequency for } D_2 = D_3 = 0}$$

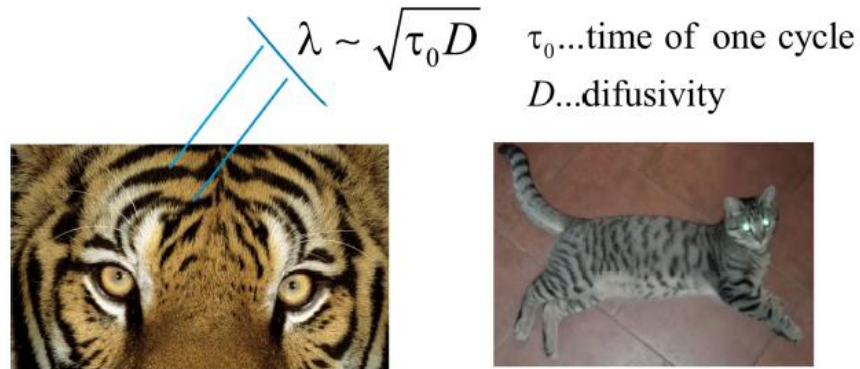
Distribution of population (concentration) e.g., of specie N_2

$$N_2 = N_{20} + \underbrace{\delta N_2 \exp(\omega_D t)}_{\text{change in time}} \exp \left\{ i \underbrace{\left[\pm \omega_D \left(\sqrt{\left(\frac{\omega_0}{\omega_D}\right)^2 - 1} \right) t - kr \right]}_{\text{traveling wave}} \right\}$$

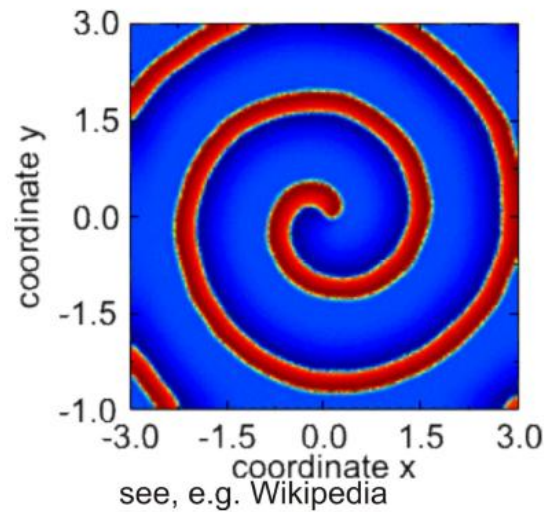
The traveling wave stops for $\omega_0 = \omega_D$ and periodic strips appear. Wave vector $k = 2\pi/\lambda$, where λ is the wavelength.

$$\lambda = \pi \sqrt{\frac{2(1+m)D_2}{\omega_0}} = \pi \sqrt{\frac{2(1+m)D_2}{\sqrt{k_{+2}N_{20}N_{30}}}} \quad m \in (-\infty, \infty)$$

An example of reaction-diffusion processes in biological systems



Two component reaction-diffusion system of
Fitzhugh-Nagumo type
...propagation of el. potential in the heart ventricles



Muscle contraction

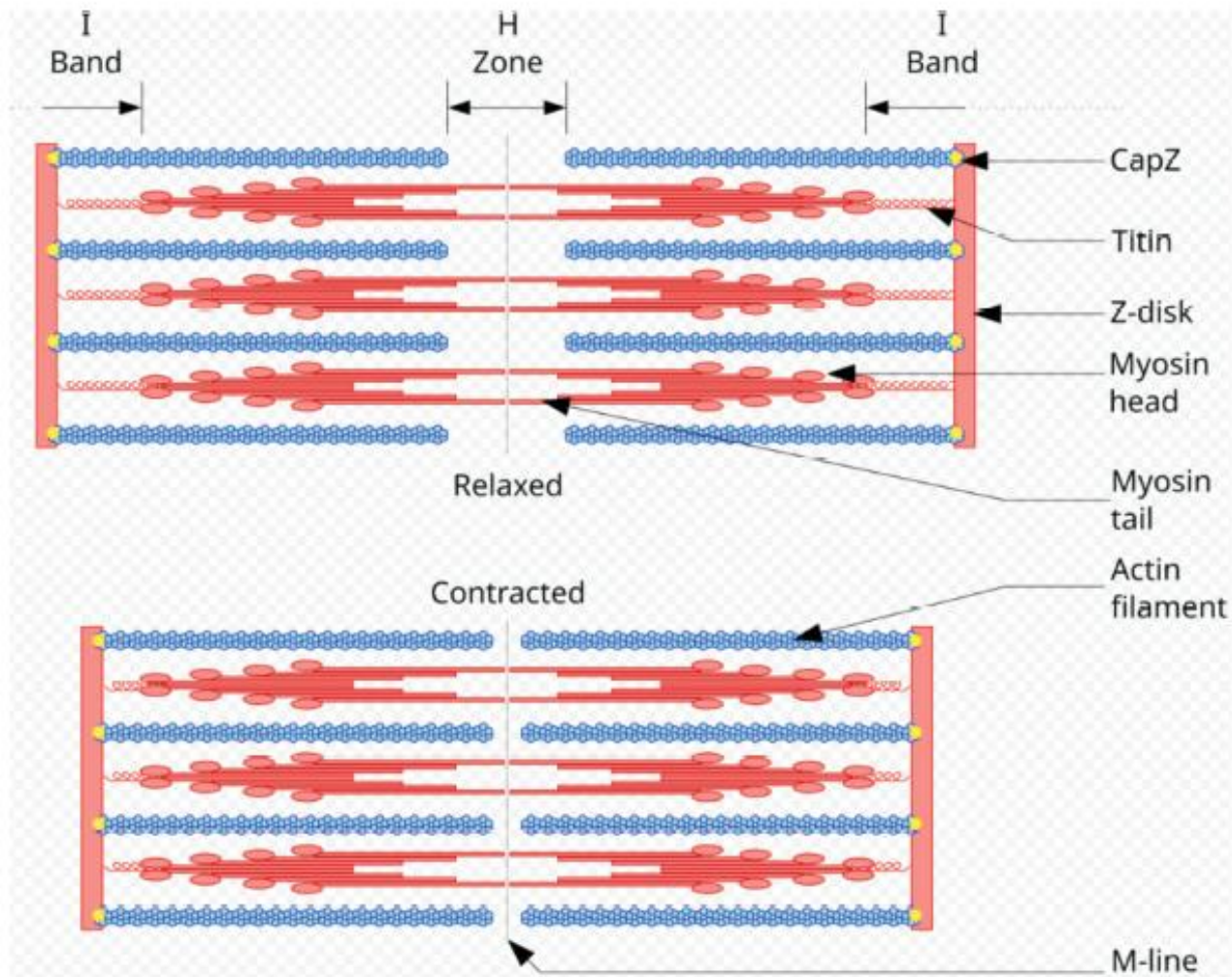
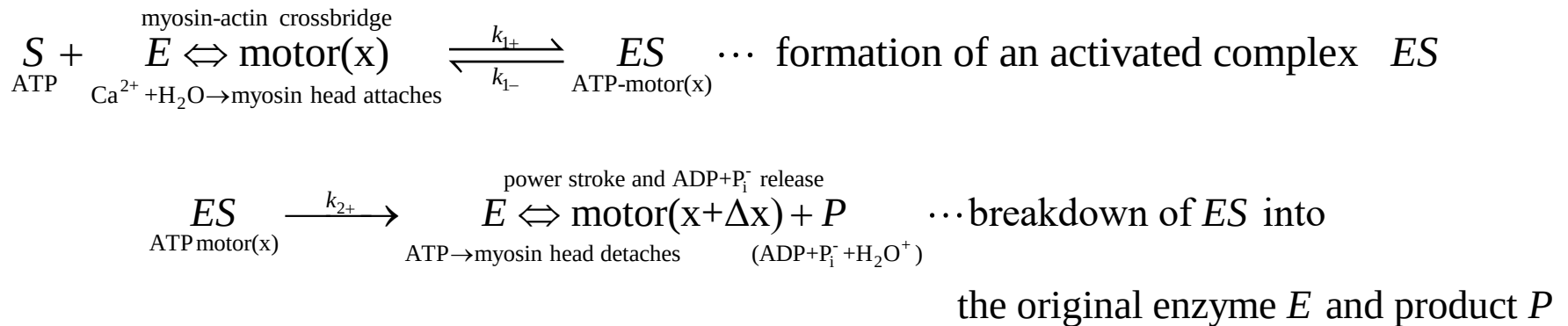


Fig. 5.1 Sliding filament concept of the muscle contraction. A sarcomere in relaxed (above) and contracted (below) positions. see Wikipedia.

Muscle contraction as a function of a molecular motor

Menten-Michaelis kinetics can be used to model muscle contraction, which can be interpreted as a molecular motor. This mechanism can be described by the following chemical kinetics

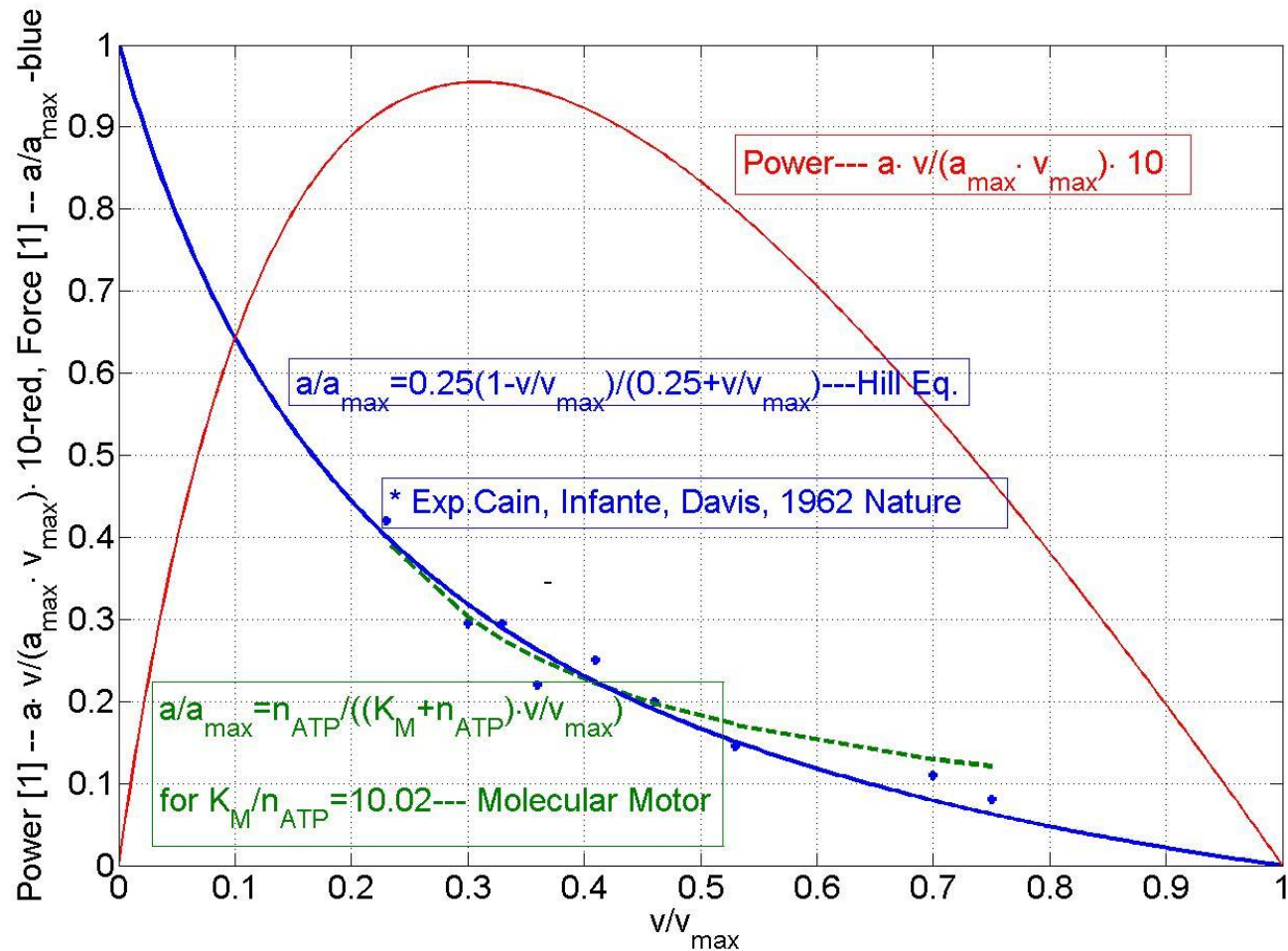


for $\Delta G = -30 \text{ kJmol}^{-1}$, $\Delta H = -20 \text{ kJmol}^{-1}$ $\Delta S = -34 \text{ Jmol}^{-1}\text{K}^{-1}$

and for human body temperature $T = (273.15 + 37) \text{ K}$, $T\Delta S = 10.5 \text{ kJmol}^{-1}\text{K}^{-1}$

Proper muscle function is ensured under conditions of stability

$$\frac{(\delta n_\alpha)^2}{n_{\alpha 0} n_{tot}} \geq_{t \gg t_0} \frac{2j_{D_\alpha}(S_0)}{\Sigma_\alpha(S) R_0}$$



Basal metabolism for woman 75 kg, 40 years old, 175 cm tall

The heat power (approximately 75 W) determines amount of consumed energy (glucose)

$$\overline{\dot{\Delta Q}}(-75\text{W}) = -\overline{\dot{\Delta G}} \text{ up to } 5 \text{ mg kg}^{-1}\text{min}^{-1} \text{ of glucose}$$

→ basal metabolism 6315 kJ day per day
equivalent 8 beers Kozel 10°

Value of basal metabolism 6315 kJ per day is used as an assumed limit value. The entropy production of a human being in basal metabolism state at ambient temperature 18°C is given from the stability condition of the dynamical equilibrium.

$$P(S_0) \sim -\frac{\overline{\dot{\Delta Q}}}{273 + 18} - \frac{\overline{\dot{\Delta G}}}{273 + 37} = 0.5 \text{WK}^{-1} < -\int_{t_1}^{t_2} \mathcal{J}(S_0) dt$$

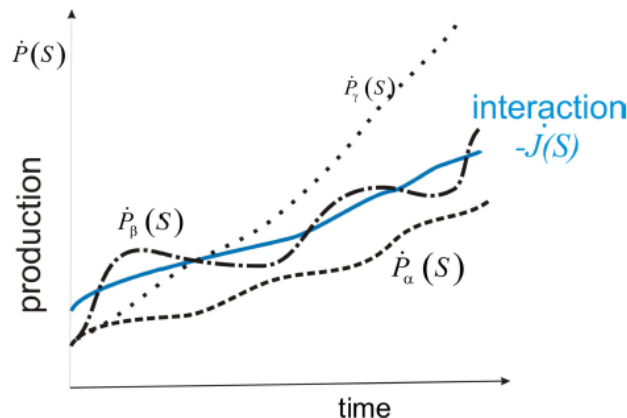
This minimal entropy production needs to be maintained by **negative entropy flux** for keeping the thermodynamic **non-equilibrium** (figuratively "**preservation of life**") and depends strongly on temperature of surroundings.

Summary for the evolution of the open systems with respect to interactions with surroundings.

- ▶ The driving force of evolution is the struggle for space and resources.
- ▶ The existence of an open system is guaranteed by its stability.
- ▶ The stability is guaranteed by system growth (extensive and intensive).

Stability condition for open system

$$\ddot{S}_0 = \dot{J}(S_0) + \dot{P}(S_0) < 0 - \text{stable evolution (or } > 0 - \text{unstable evolution)}$$



$\dot{P}_\alpha$ – stable evolution,
 $\dot{P}_\beta$ – dynamic evolution,
 $\dot{P}_\gamma$ – unstable evolution.

Who knows the true future state of the system?

- where is the truth --- only God knows the truth (G.W.F. Hegel *1770)
 - are the laws of evolution the laws of God?
 - does evolution have anything to do with God?
-
- Everyone has to answer for themselves
 - Everyone is largely responsible for their own development - destiny.

Thank you for your attention and I wish you good luck on
your journey to the truth.

It is said that moderate wine consumption helps with this.



I'm always a little embarrassed by your wine, František. It reminds me partly
of a 1930 Bordeaux and partly of ant poison.

*Dein Wein ist mir immer etwas peinlich, František. Er erinnert mich teils an einen
Bordeaux von 1930 und teils an Ameisengift.*