Onset of natural selection and “Reversal of the Second Law”

Alexei V. Tkachenko

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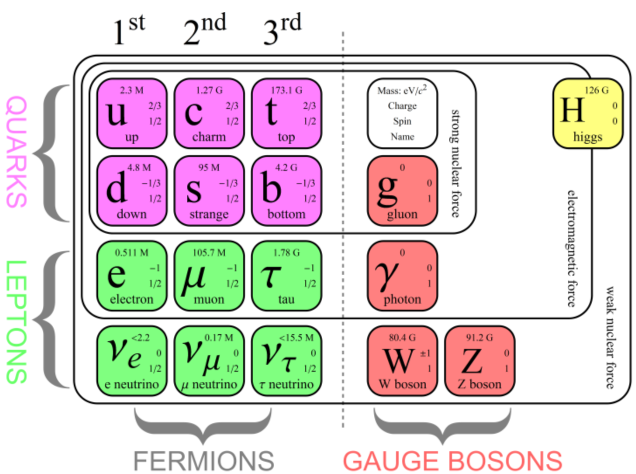
More is Different

P.W. Anderson, Science, 177, 4047 (1972)



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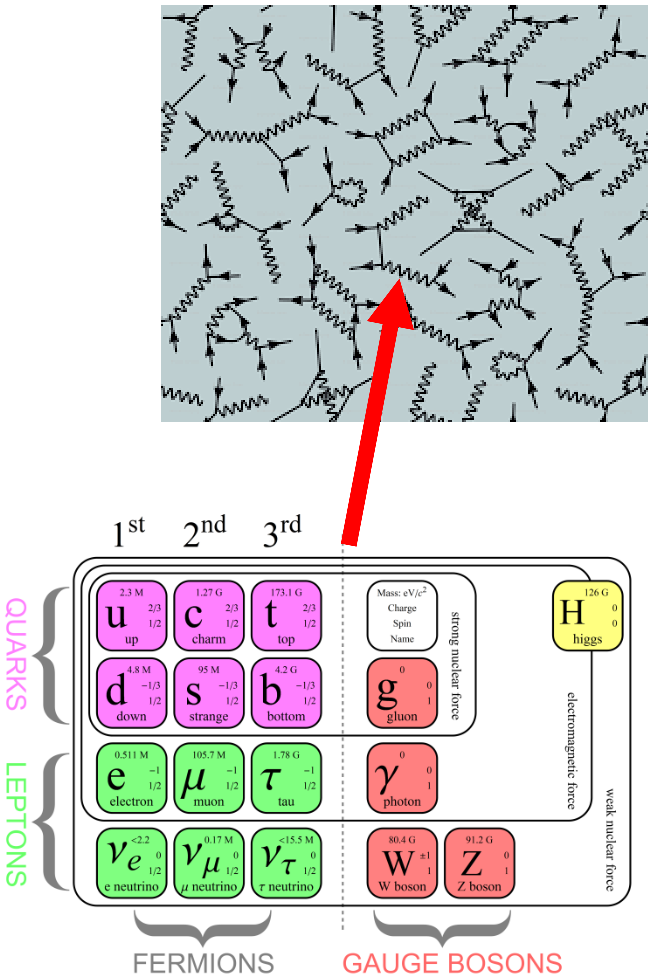

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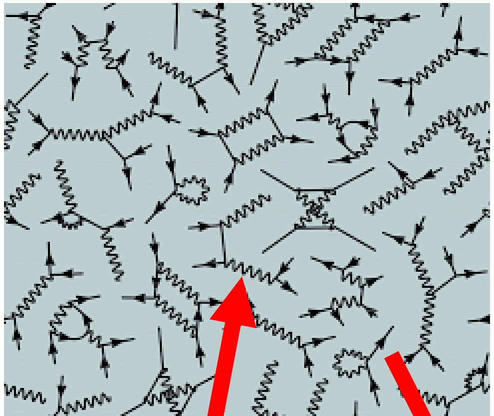

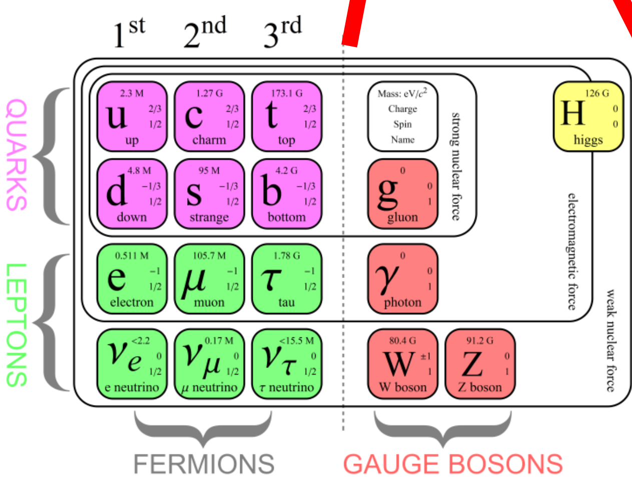

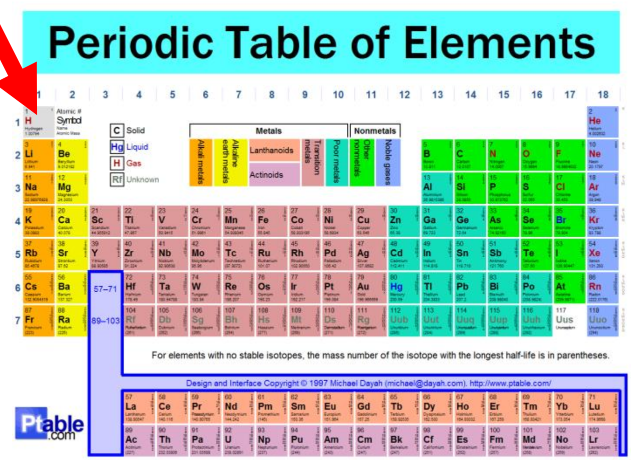

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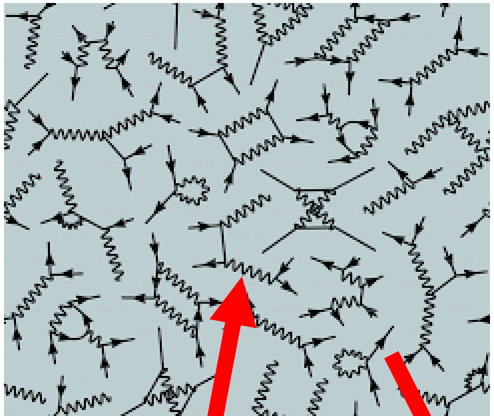

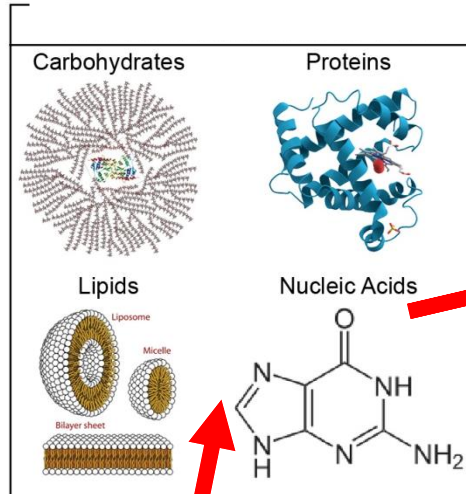

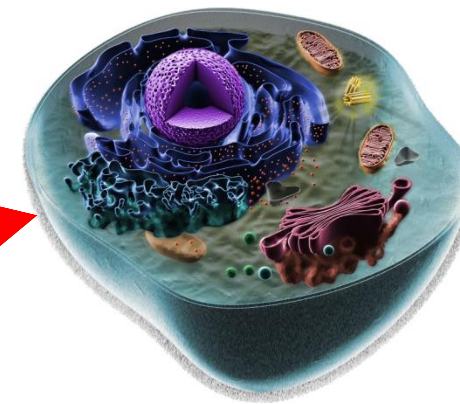

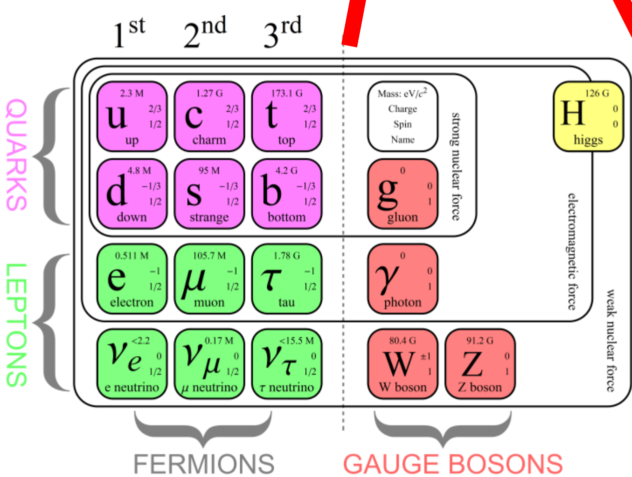

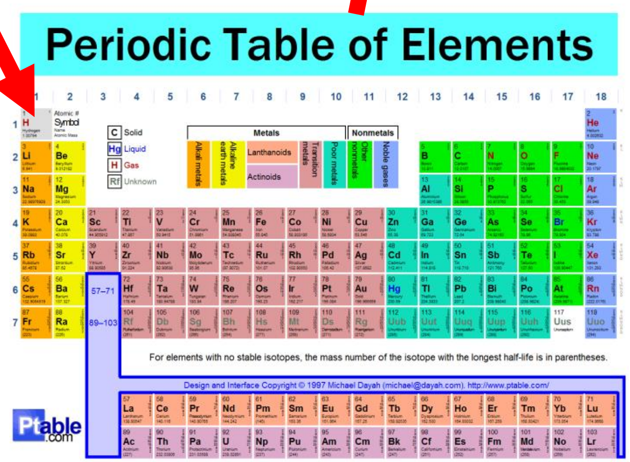

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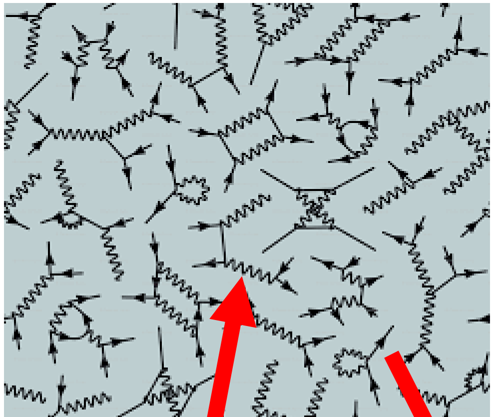

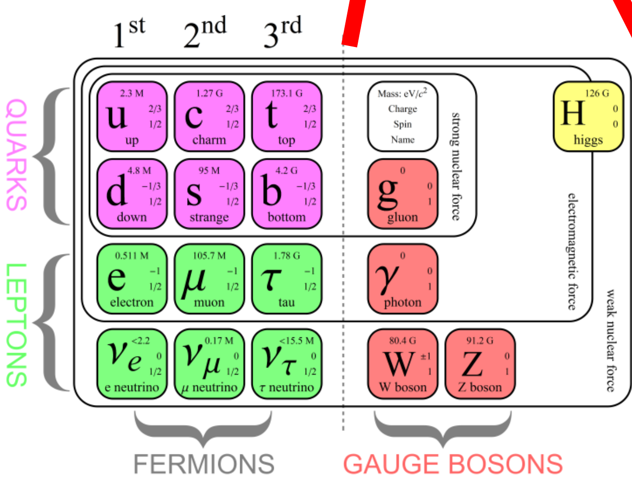

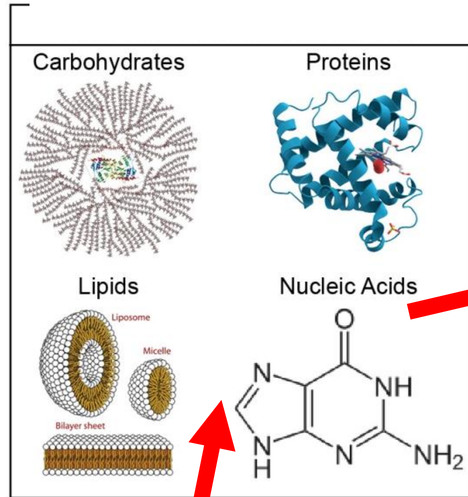

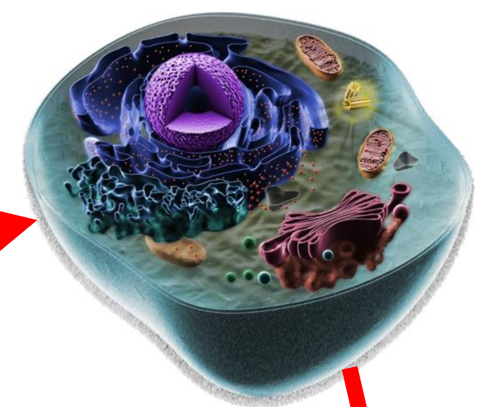

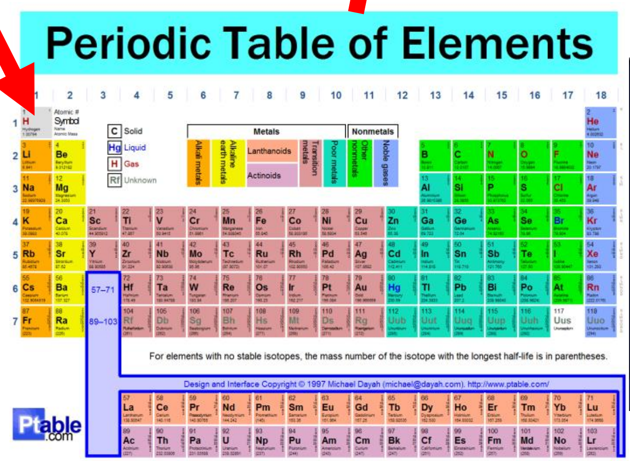

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- How does **Thermodynamics** emerge from **Mechanics**?
- How does **Classical** domain emerge in **Quantum Theory**?
- How does **Life** emerge form **non-living Matter**?
- How does **Consciousness** emerge?

…these are the questions

- How does **Thermodynamics** emerge from **Mechanics**?
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- How does **Consciousness** emerge?

All these questions are related to

Entropy *&* ***Information***

<u>Needed:</u> the simplest Darwinian system

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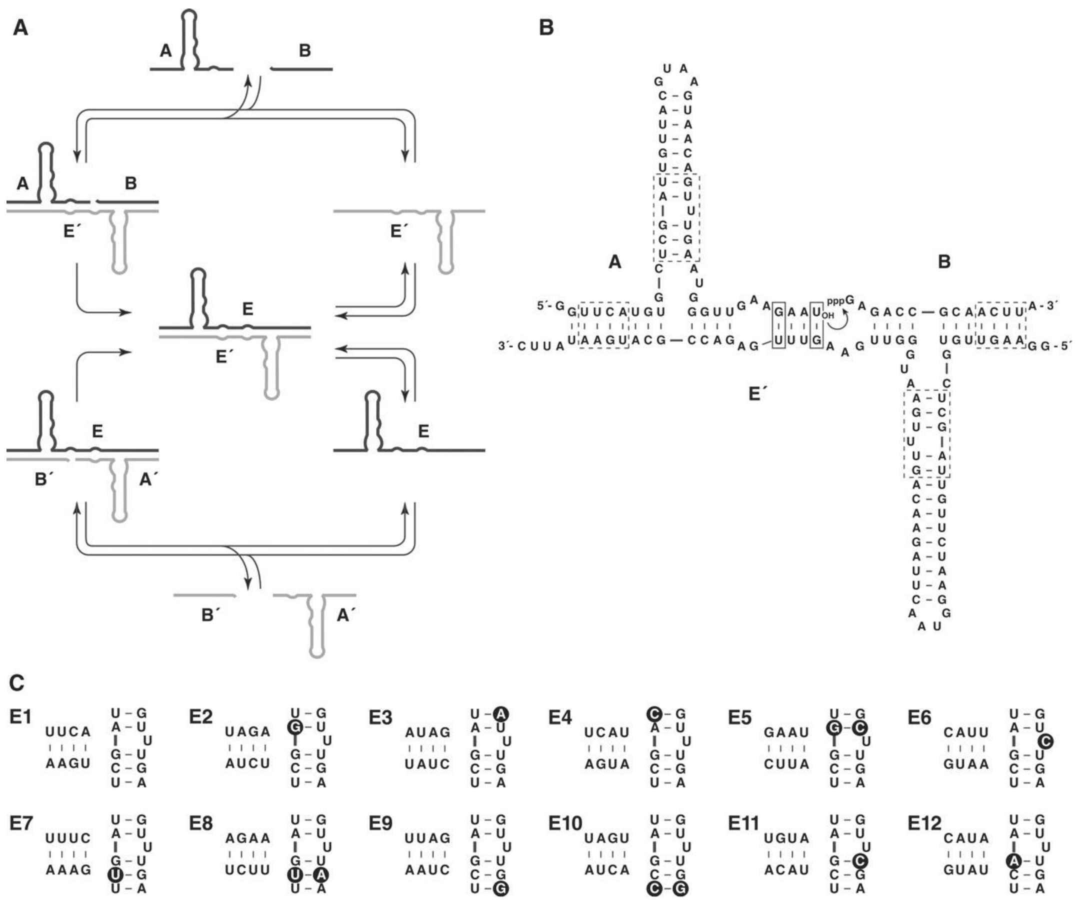
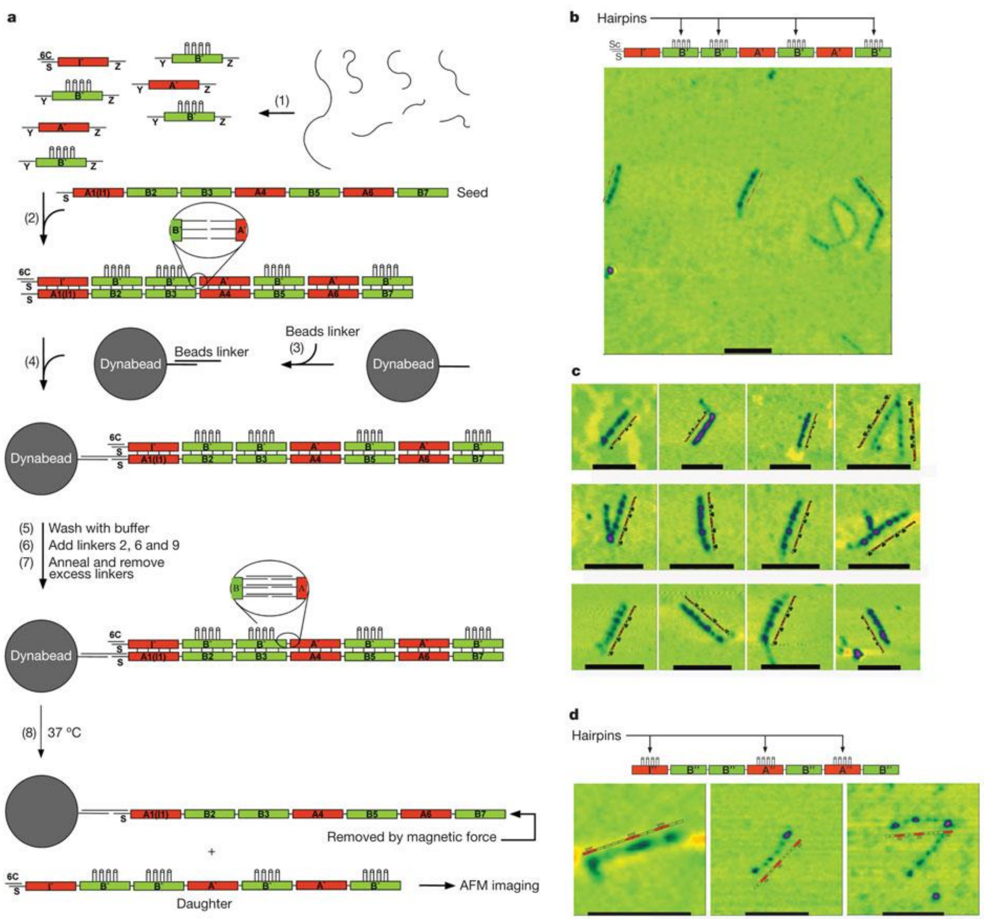
RNA world: Self-replication of RNA Enzymes



T. A. Lincoln, G.F. Joyce, Science 323, 1229 (2009)

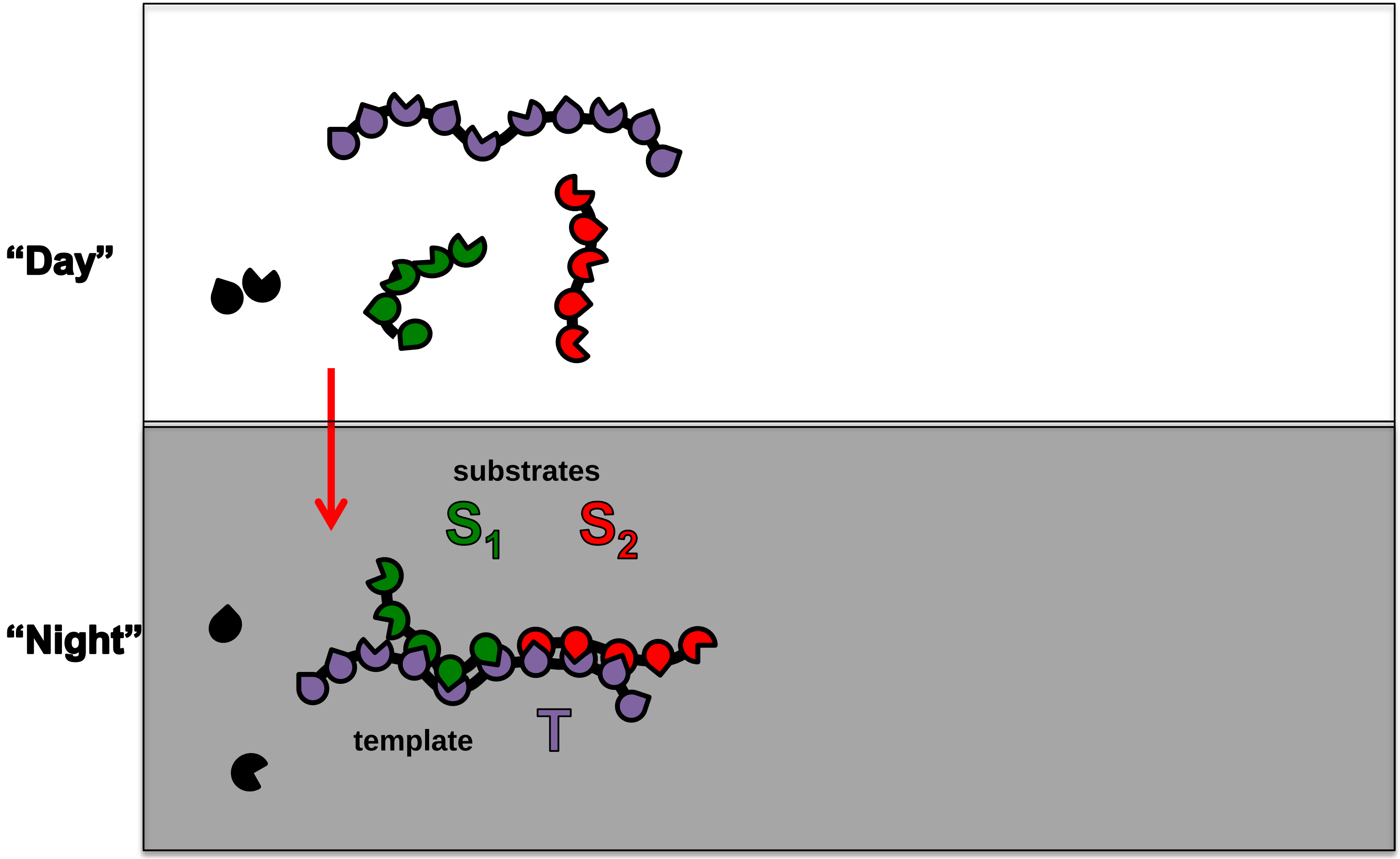
Self-replication Based on DNA Origami



T Wang *et al. Nature* 478, 225-228 (2011)

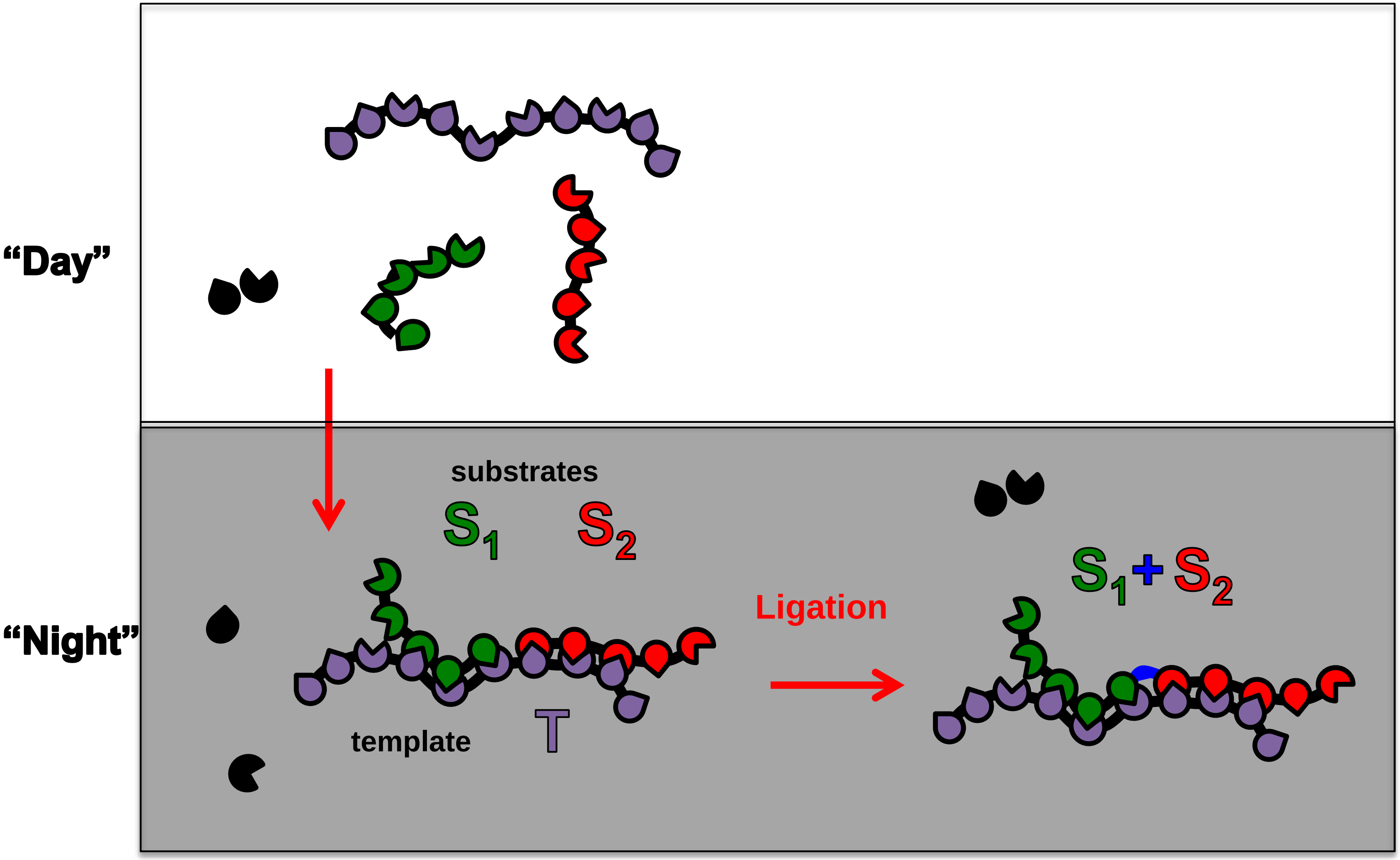
Template-Assisted Ligation

(with Sergei Maslov, UIUC)

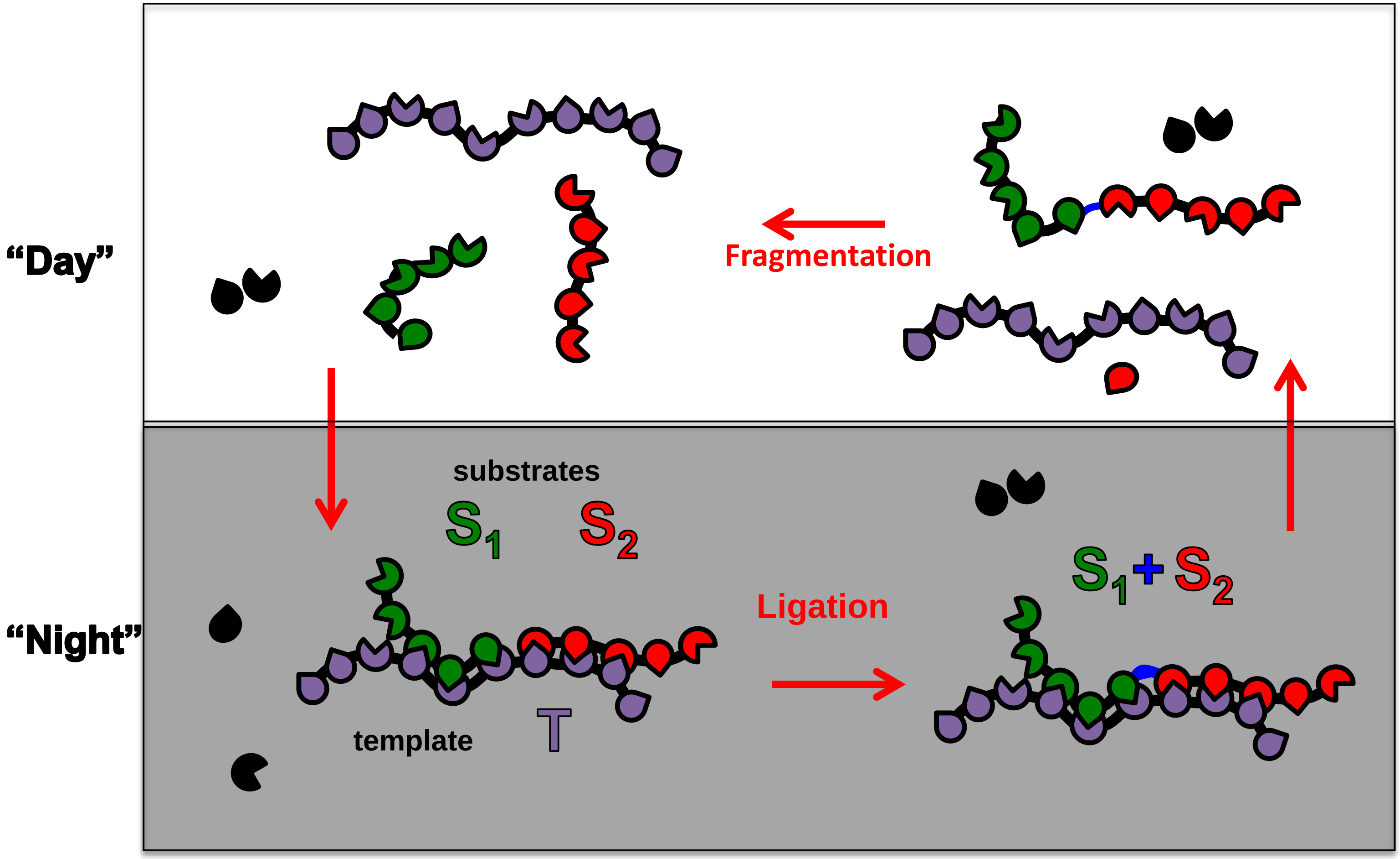


Model inspired by: *P. W. Anderson,* Proc. Natl. Acad. Sci. USA. 80, 3386 (1983).

Template-Assisted Ligation

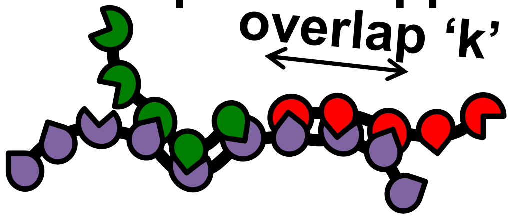


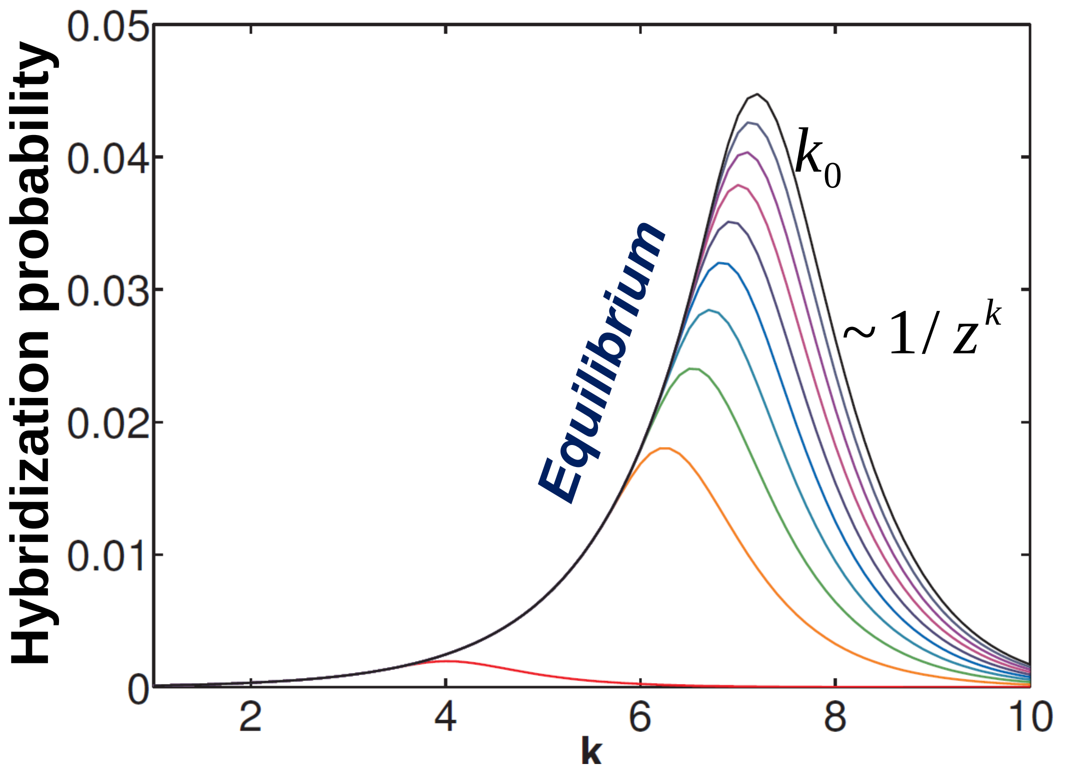
Template-Assisted Ligation



Optimal overlap length

We start with Random Sequence Approximation



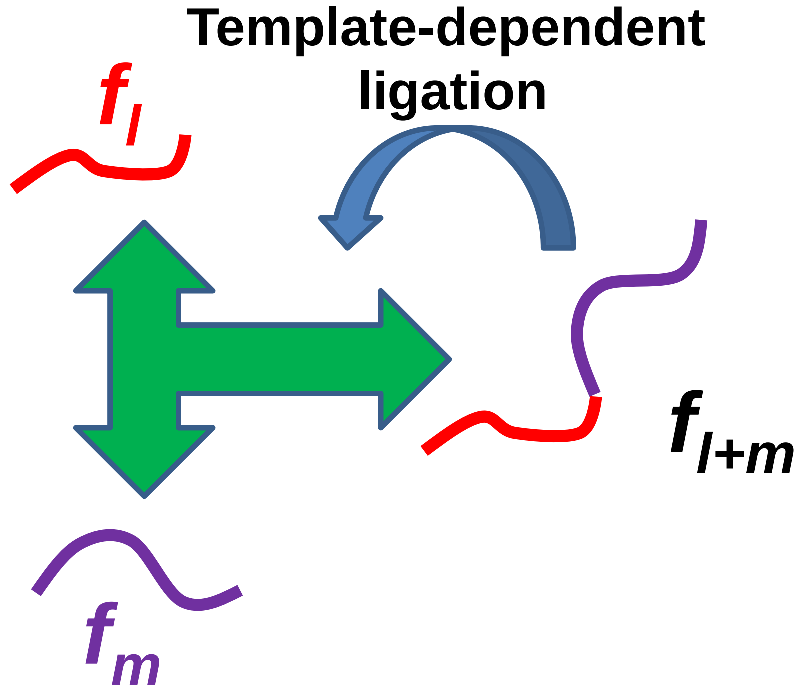


Analytic theory

β – fragmentation rate
λ – ligation rate

For $l,m>k_0$: detailed balance.

$$f_l \sim \exp\left(-l/\bar{L}\right), \quad l > k_0$$

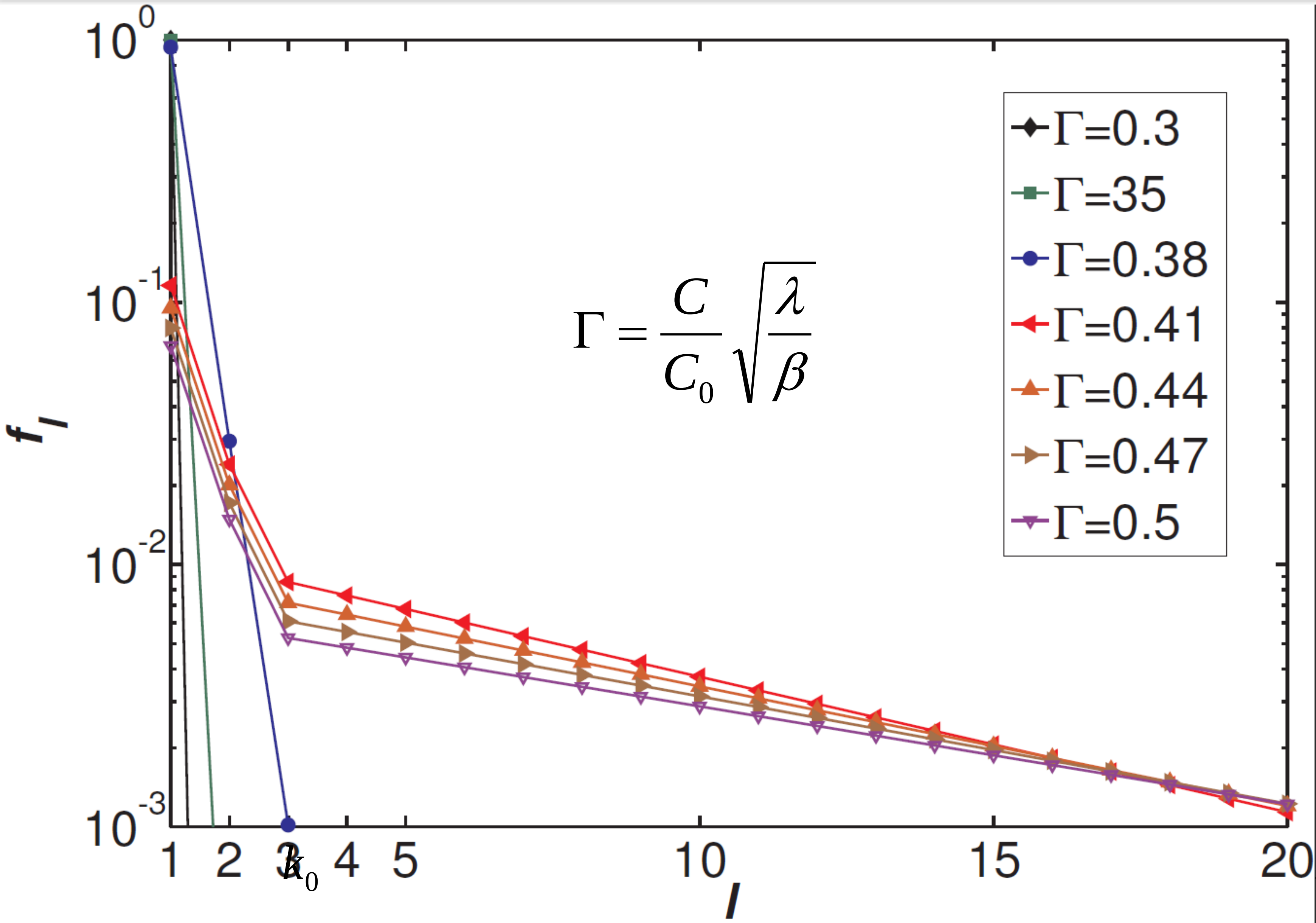


The autocatalytic pool of long chains emerges via 1st order transition:

$$C \sim C_0 \sqrt{\frac{\beta}{\lambda}}$$

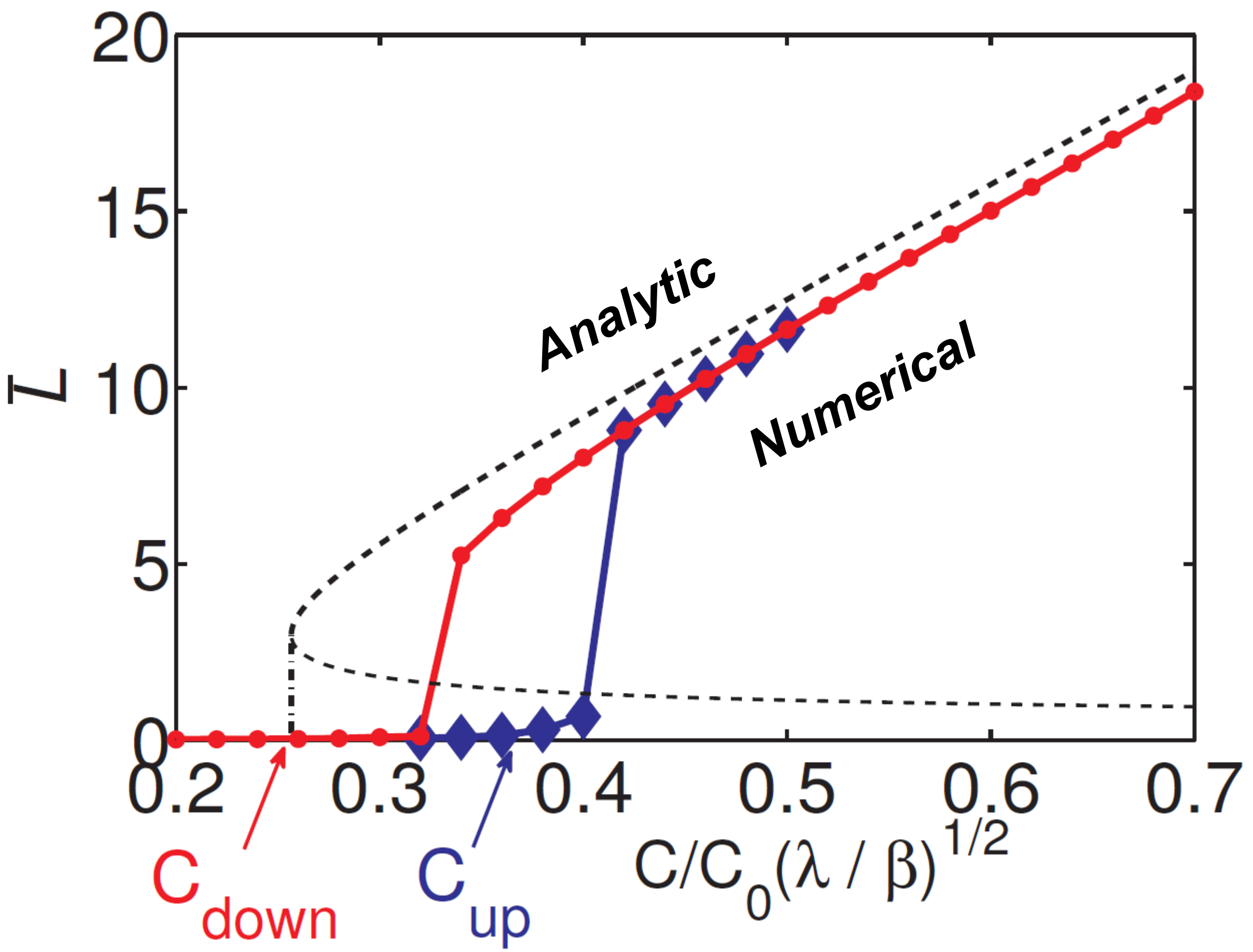
- minimal monomer concentration

Chain Length Distribution (numerical)



First Order Transition

AV Tkachenko & S Maslov, J. Chem. Phys. 143, 045102 (2015)



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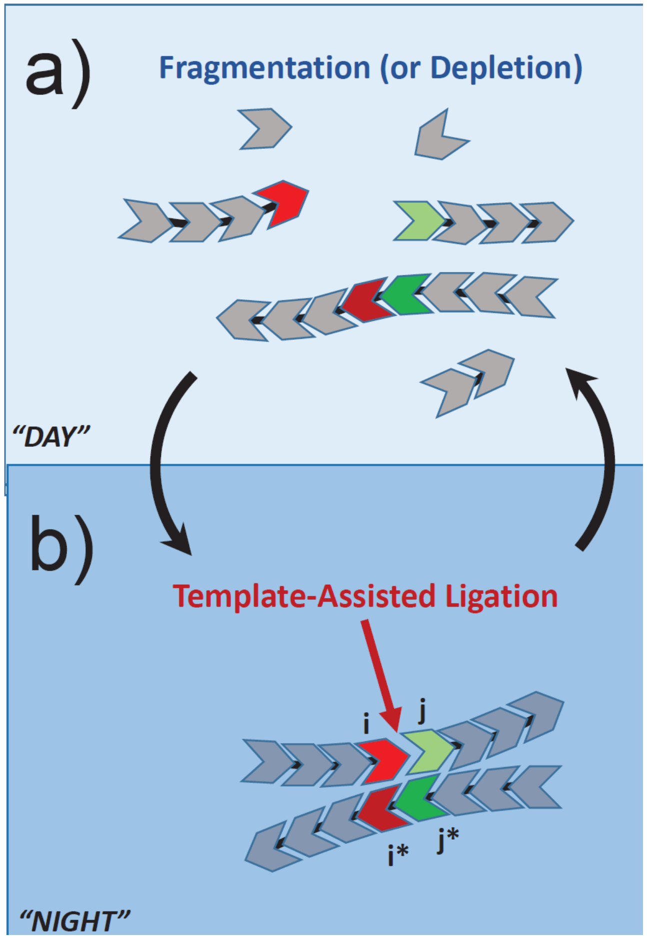
What about sequences?



$$A^{(right)} + B^{(left)} \xrightarrow[\uparrow\; B^*A^*]{} AB$$

Let <u>any pair of consecutive letters</u> (“doublet”), work as a template for ligation:

$$\dot{d}_{ij} = \lambda_{ij} l_i r_j d_{j^*i^*} - \beta_{ij} d_{ij}$$

$$l_i + \sum_j d_{ij} = r_i + \sum_j d_{ji} = C_i \quad \text{(monomer conservation)}$$

i is complementary to i (i,j,i*,j* =1…Z).*
d_{ij} – density of “doublets”, pairs of given consecutive letters anywhere in the pool.
l_i, r_j – density of “left” and “right” chain ends terminated with “i”
l_{ij} and b_{ij} are ‘ligation’ and ‘fragmentation’ rates.

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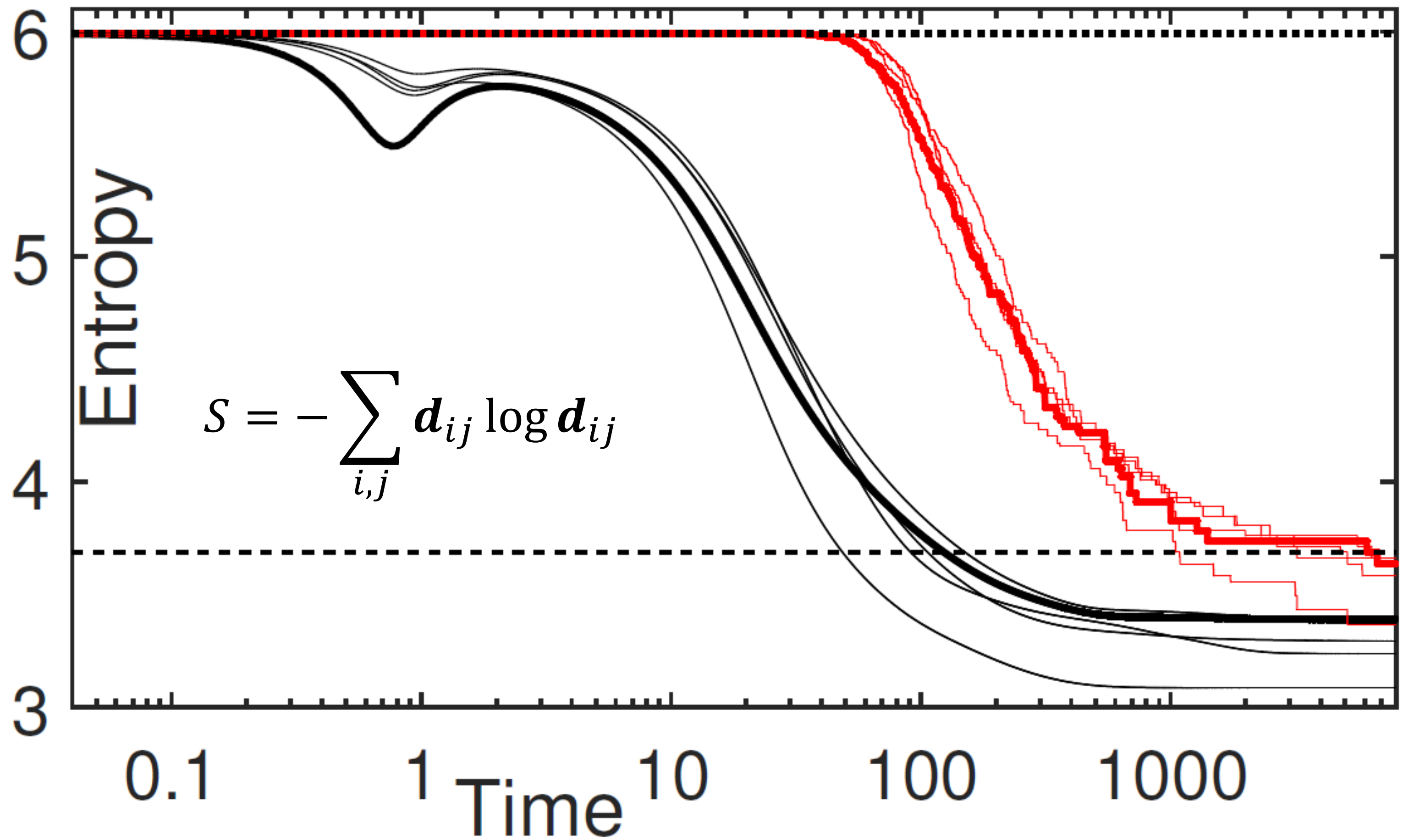
Information Entropy decreases!



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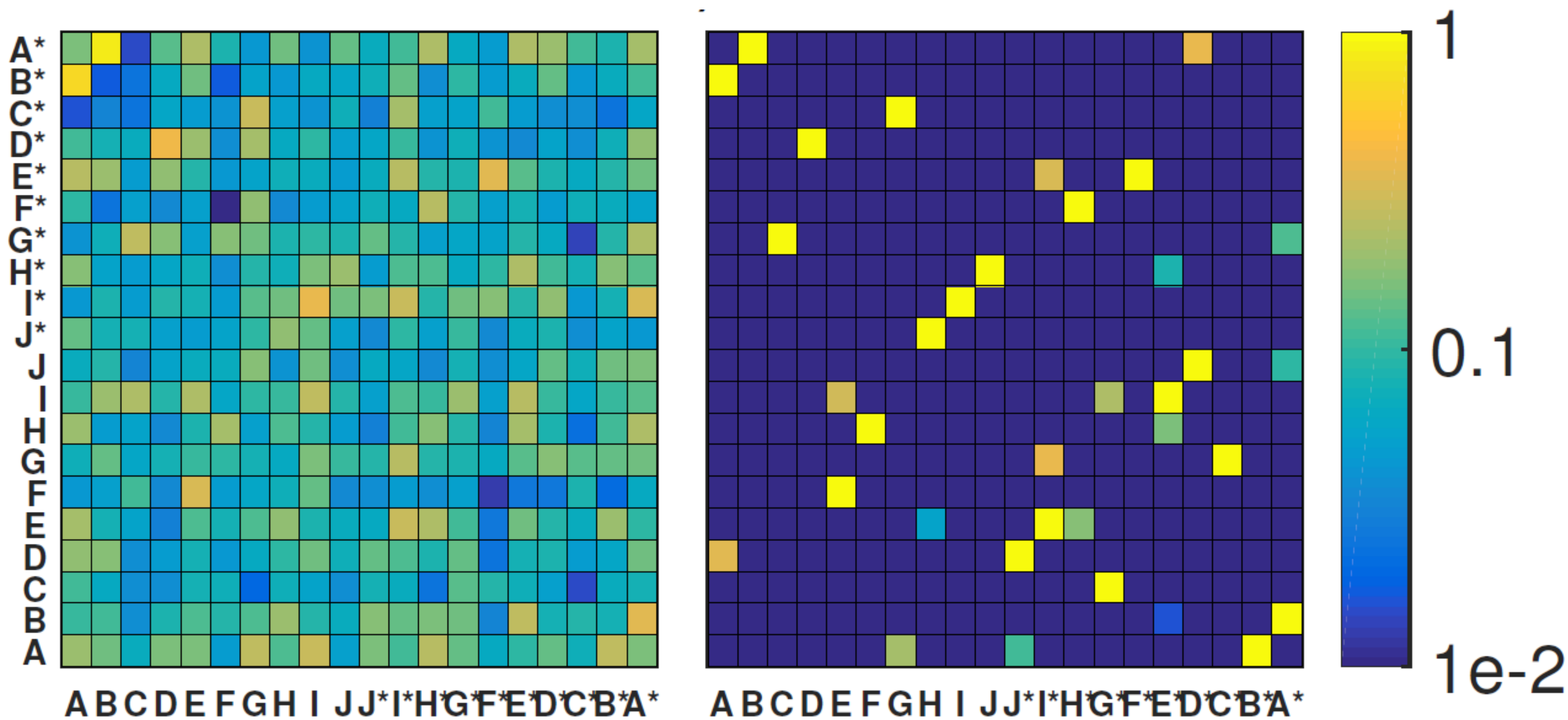
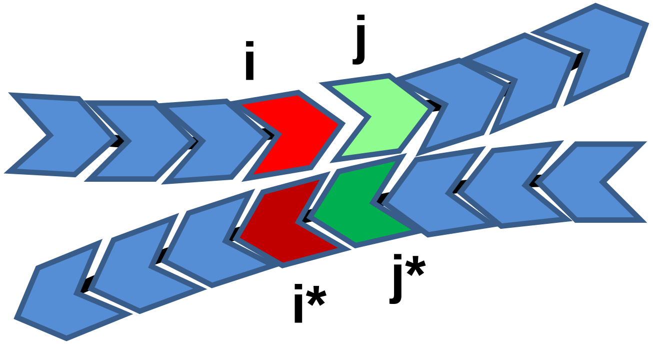
Evolved "doublet" matrix



Survivor game



$$\frac{\partial}{\partial t}\begin{bmatrix} d_{ij} \\ d_{j^*i^*} \end{bmatrix} = \begin{bmatrix} -1 & \lambda_{ij} r_i l_j \\ \lambda_{j^*i^*} r_{j^*} l_{i^*} & -1 \end{bmatrix} \begin{bmatrix} d_{ij} \\ d_{j^*i^*} \end{bmatrix}$$

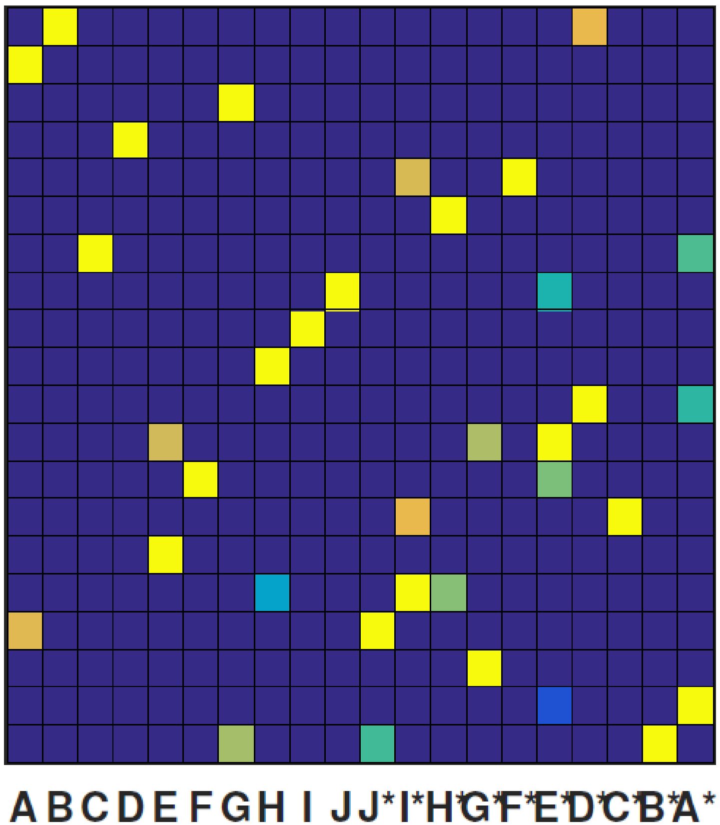
$$-\det = \lambda_{ij}\lambda_{j^*i^*}(r_i l_{i^*})(r_{j^*} l_j) - 1 \rightarrow \begin{cases} > 0: & \text{growing} \\ = 0: & \text{steady} \\ < 0: & \text{"extinct"} \end{cases}$$

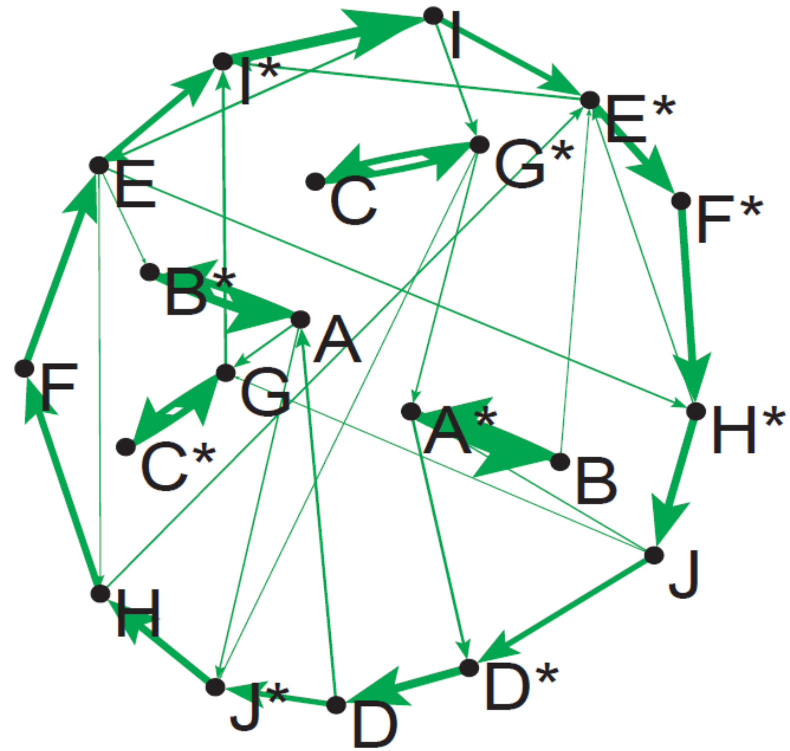
Maximum number of these equations = number of variables (**Z**)

⇩

The upper bound on number of surviving doublets is ***2Z***, *not* ***Z²***

deBruin graph representation

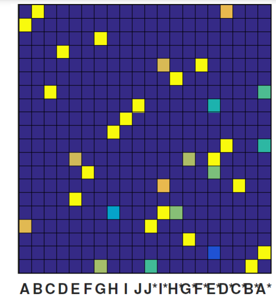




Entire sequence pool is generated as a Marcowian walk on this graph

Searching for a “better” Life

$$(C_1, C_2, \ldots\ldots, C_Z) \xrightarrow{\hat{\lambda}}$$ **unique steady state**



Multiple realizations of $\{C_i\}$ $\longrightarrow$ efficient sampling of the sequence space

What is life?

*Chromosomes … contain in some kind of **code-script** the entire pattern of the individual's future development and of its functioning in the mature state*

Life feeds on negative entropy
*The device by which an organism maintains itself stationary at a fairly high level of orderliness really consists in **continually sucking orderliness from its environment***

Erwin Schrödinger
(1887-1961)