

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

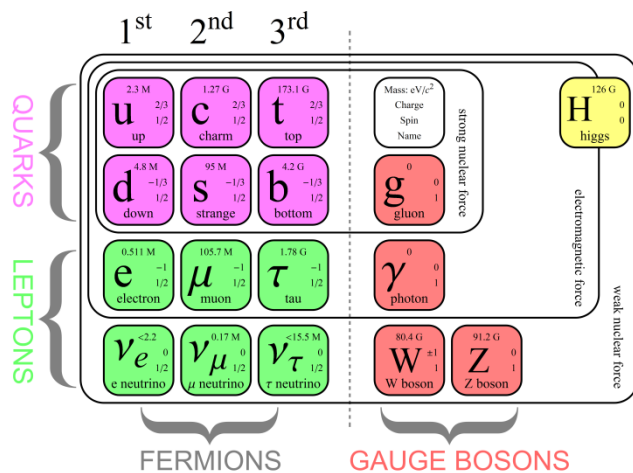
Alexei V. Tkachenko



Funding: U.S. DOE, Office of BES Contract No. DEAC0298CH10886

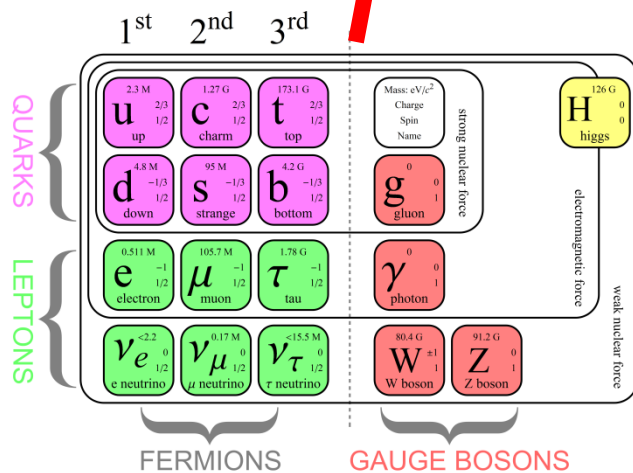
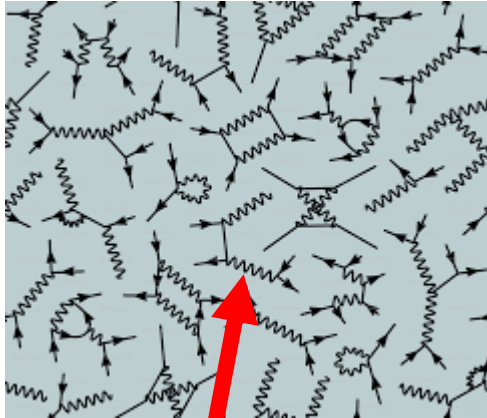
More is Different

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



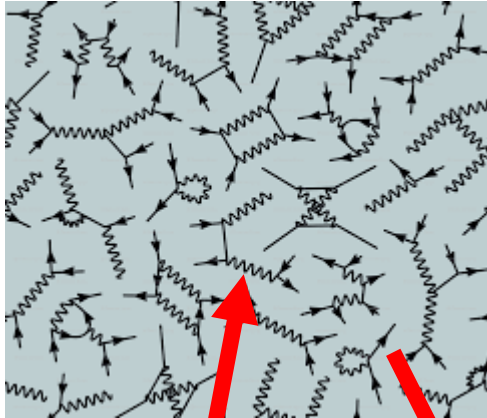
More is Different

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	1 st	2 nd	3 rd	
QUARKS	u up 2.3 M 2/3 1/2	c charm 1.27 G 2/3 1/2	t top 173.1 G 2/3 1/2	strong nuclear force g gluon 0 0 1
	d down 4.8 M -1/3 1/2	s strange 95 M -1/3 1/2	b bottom 4.2 G -1/3 1/2	
LEPTONS	e electron 0.511 M -1 1/2	μ muon 105.7 M -1 1/2	τ tau 1.78 G -1 1/2	electromagnetic force γ photon 0 0 1
	ν_e e neutrino <2.2 0 1/2	ν_μ μ neutrino 0.17 M 0 1/2	ν_τ τ neutrino <15.5 M 0 1/2	
	FERMIONS			weak nuclear force W W boson 80.4 G ±1 1
				Z Z boson 91.2 G 0 1
				GAUGE BOSONS

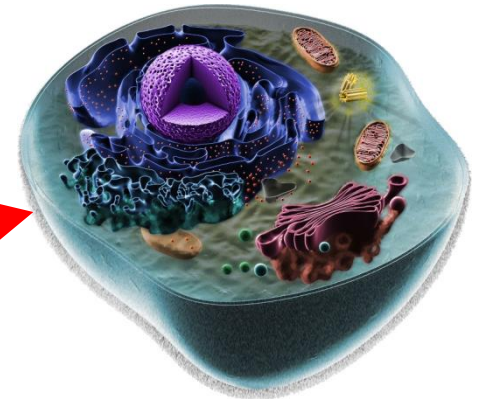
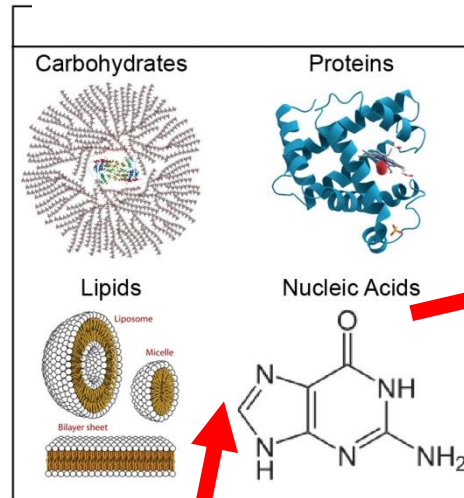
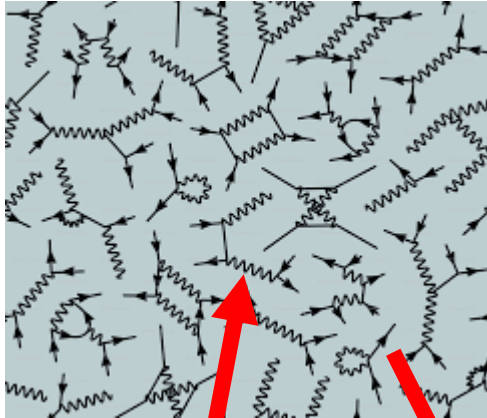
Periodic Table of Elements

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

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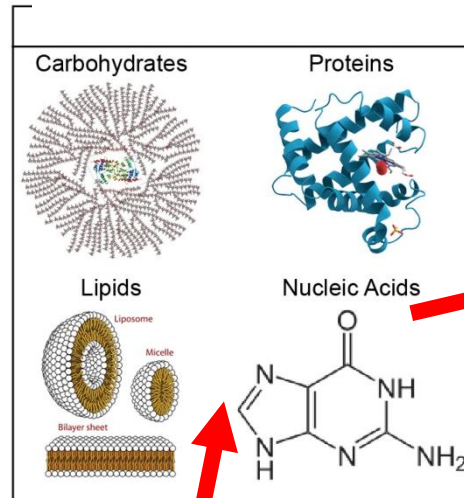
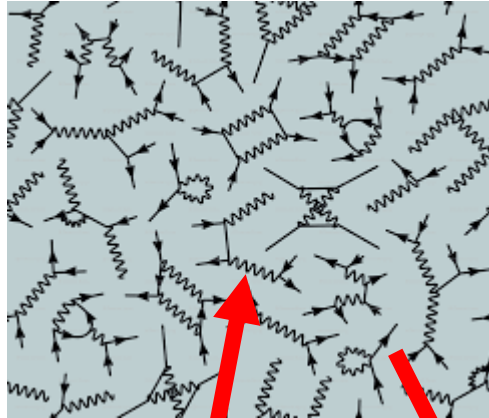
Periodic Table of Elements

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More is Different

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



	1 st	2 nd	3 rd	
QUARKS	<div>2.3 M u 2/3 up</div>	<div>1.27 G c 2/3 charm</div>	<div>173.1 G t 2/3 top</div>	<div>Mass: eV/c² Charge Spin Name</div> <div>strong nuclear force</div>
	<div>4.8 M d -1/3 down</div>	<div>95 M s -1/3 strange</div>	<div>4.2 G b -1/3 bottom</div>	<div>0 g 0 1 gluon</div>
	<div>0.511 M e -1 electron</div>	<div>105.7 M μ -1 muon</div>	<div>1.78 G τ -1 tau</div>	<div>0 γ 1 photon</div>
LEPTONS	<div><2.2 ν_e 0 e neutrino</div>	<div>0.17 M ν_μ 0 μ neutrino</div>	<div><15.5 M ν_τ 0 τ neutrino</div>	<div>80.4 G W ±1 W boson</div>
				<div>91.2 G Z 0 Z boson</div>
	FERMIONS			GAUGE BOSONS

Periodic Table of Elements

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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

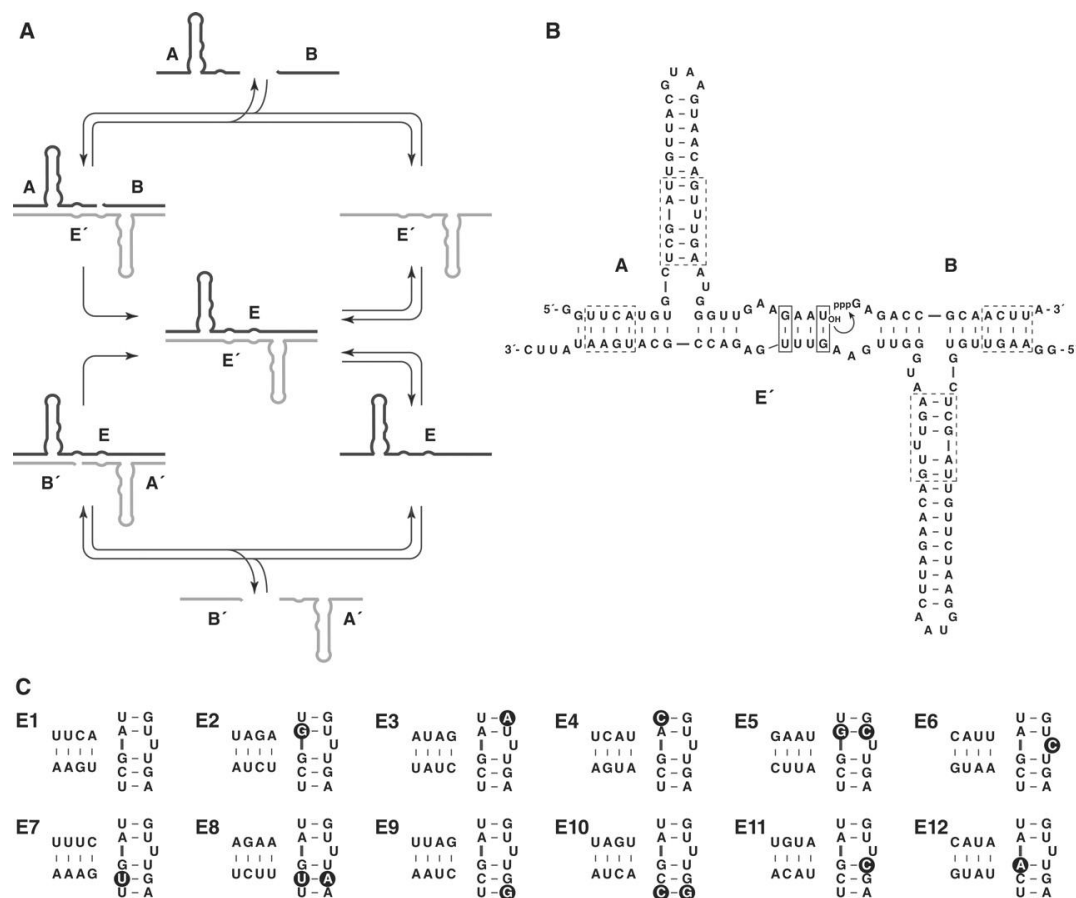
- How does Thermodynamics emerge from Mechanics?
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All these questions are related to
Entropy & Information

Needed: the simplest Darwinian system

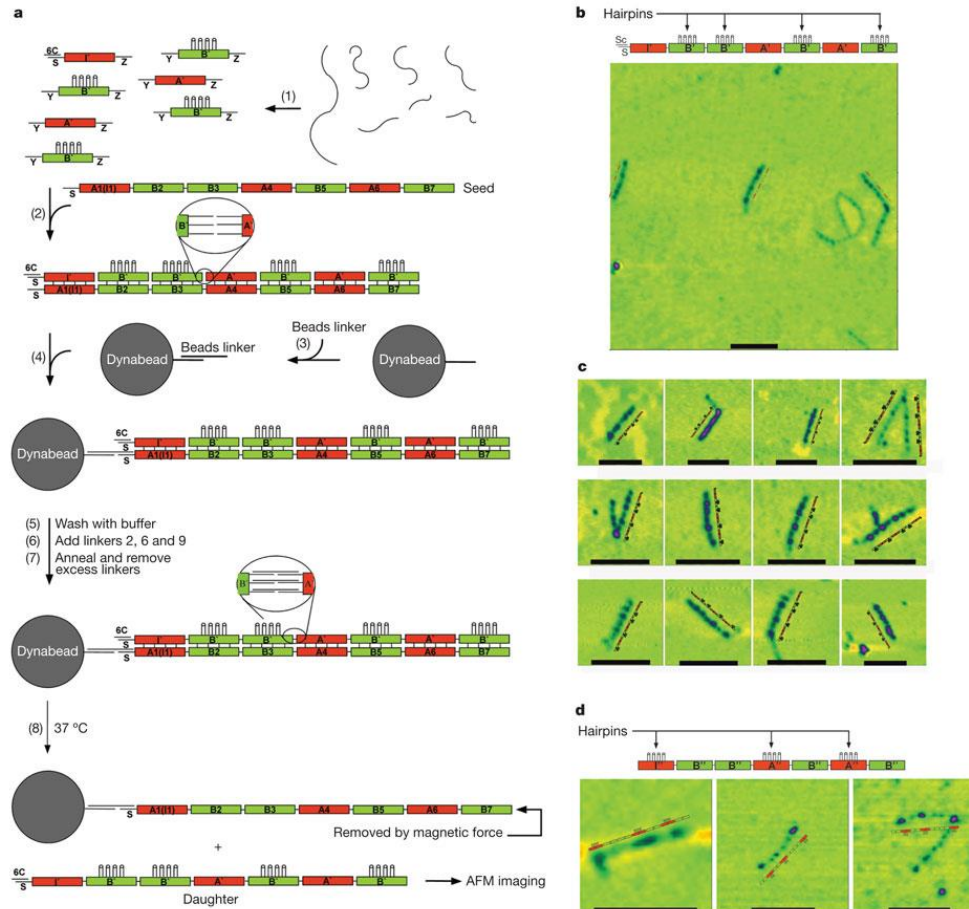


RNA world: Self-replication of RNA Enzymes



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

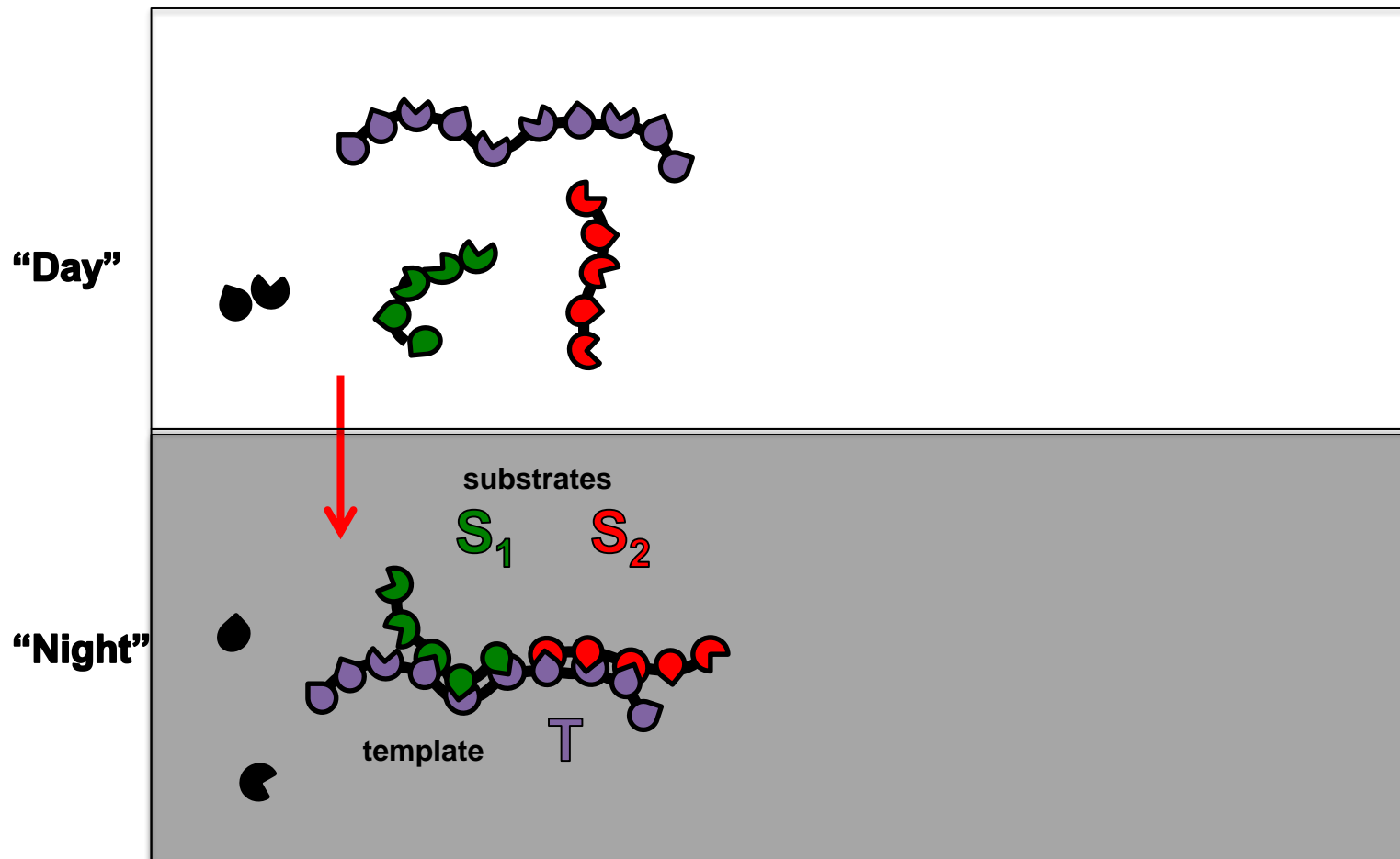
Self-replication Based on DNA Origami



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

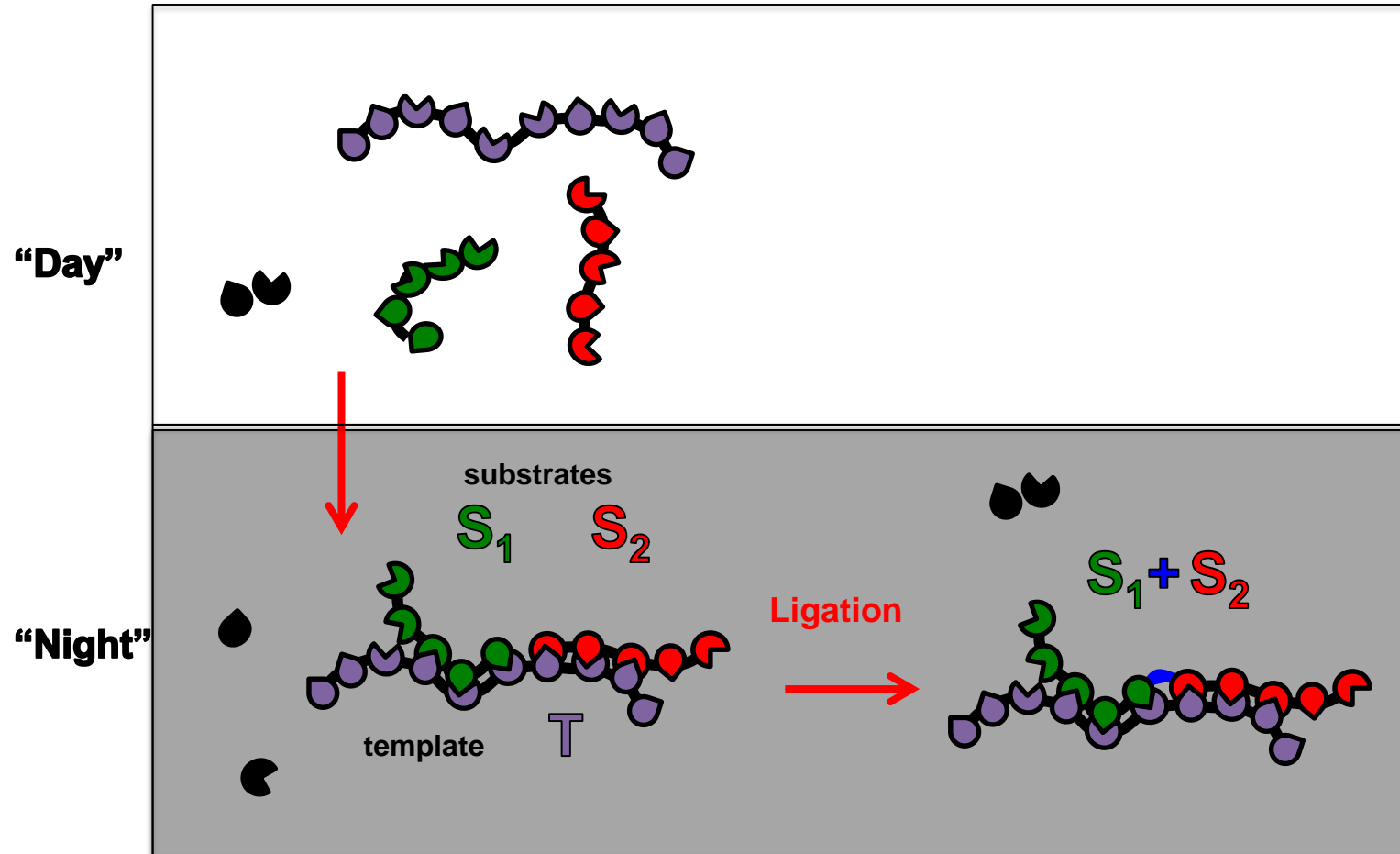
Template-Assisted Ligation

(with Sergei Maslov, UIUC)

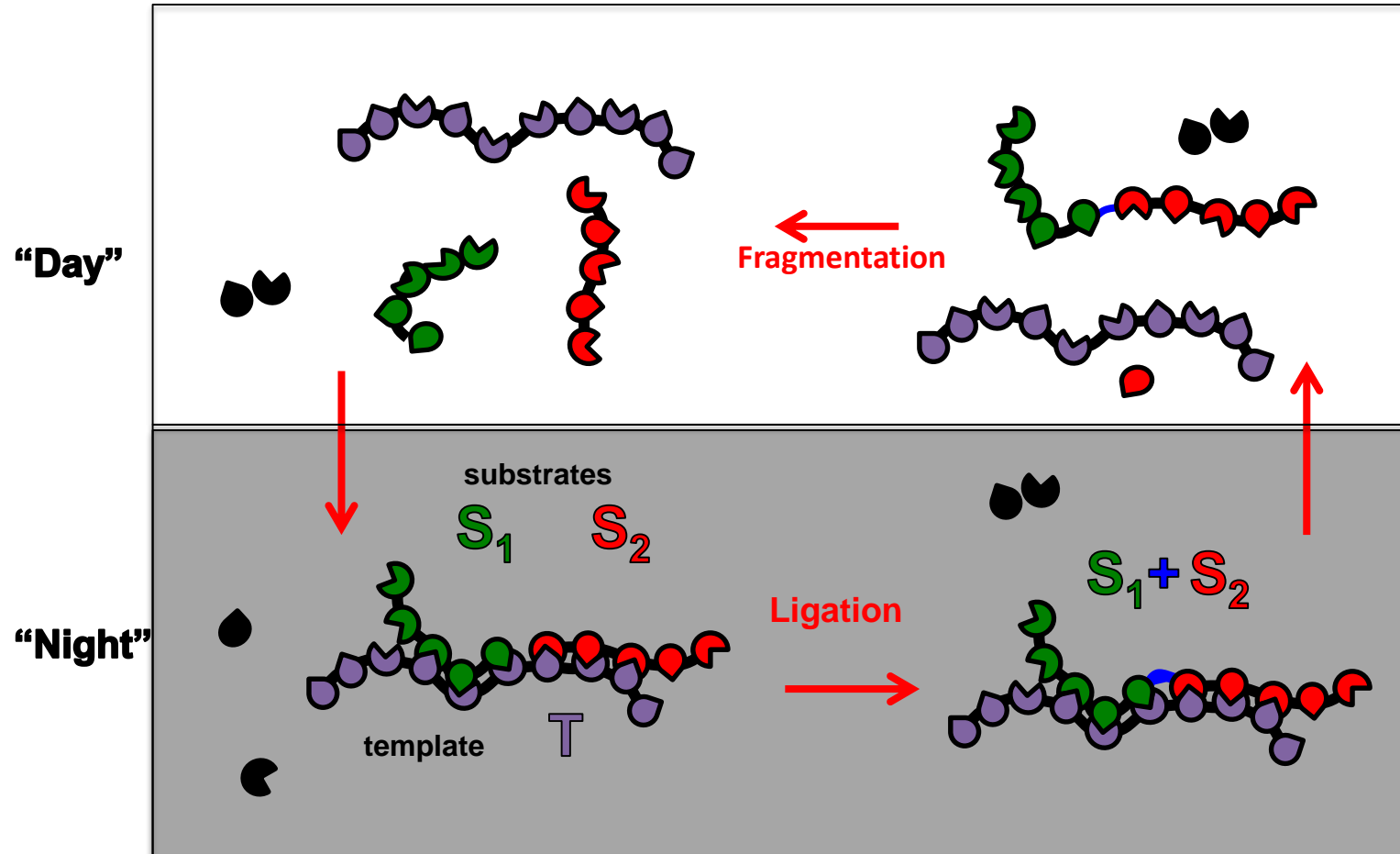


Model inspired by: *P. W. Anderson*, Proc. Natl. Acad. Sci. USA. 80, 3386 (1983).

Template-Assisted Ligation

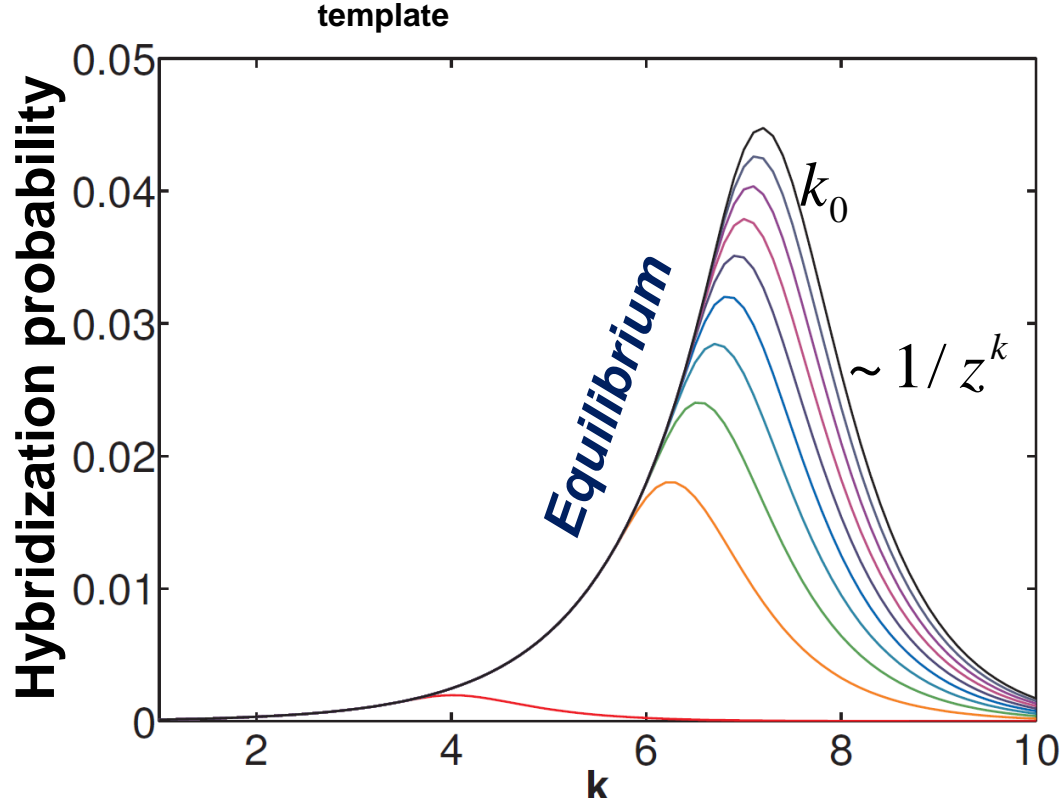
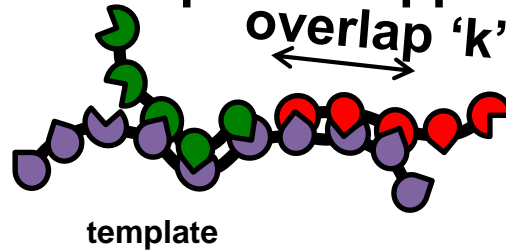


Template-Assisted Ligation



Optimal overlap length

We start with Random Sequence Approximation

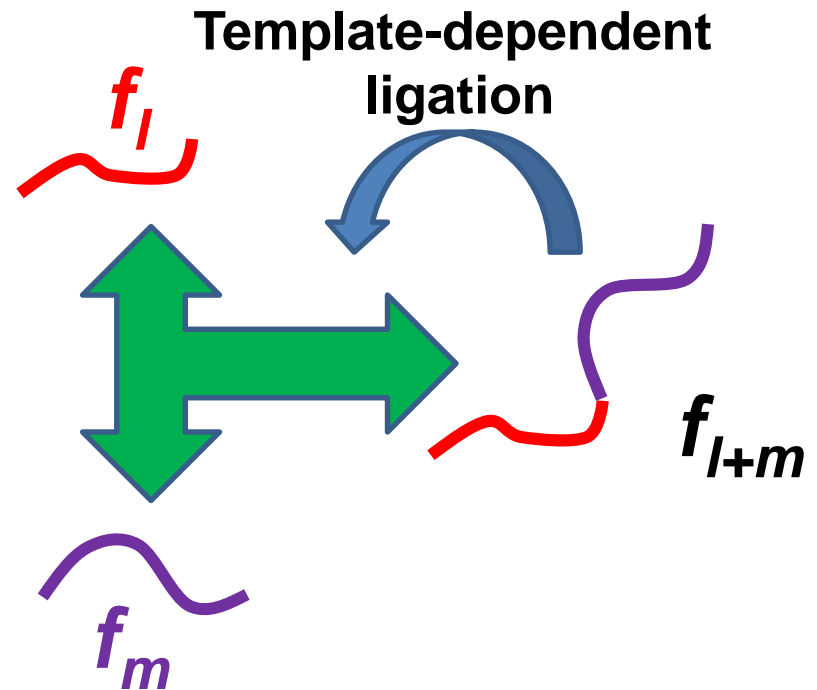


Analytic theory

β – fragmentation rate
 λ – ligation rate

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

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



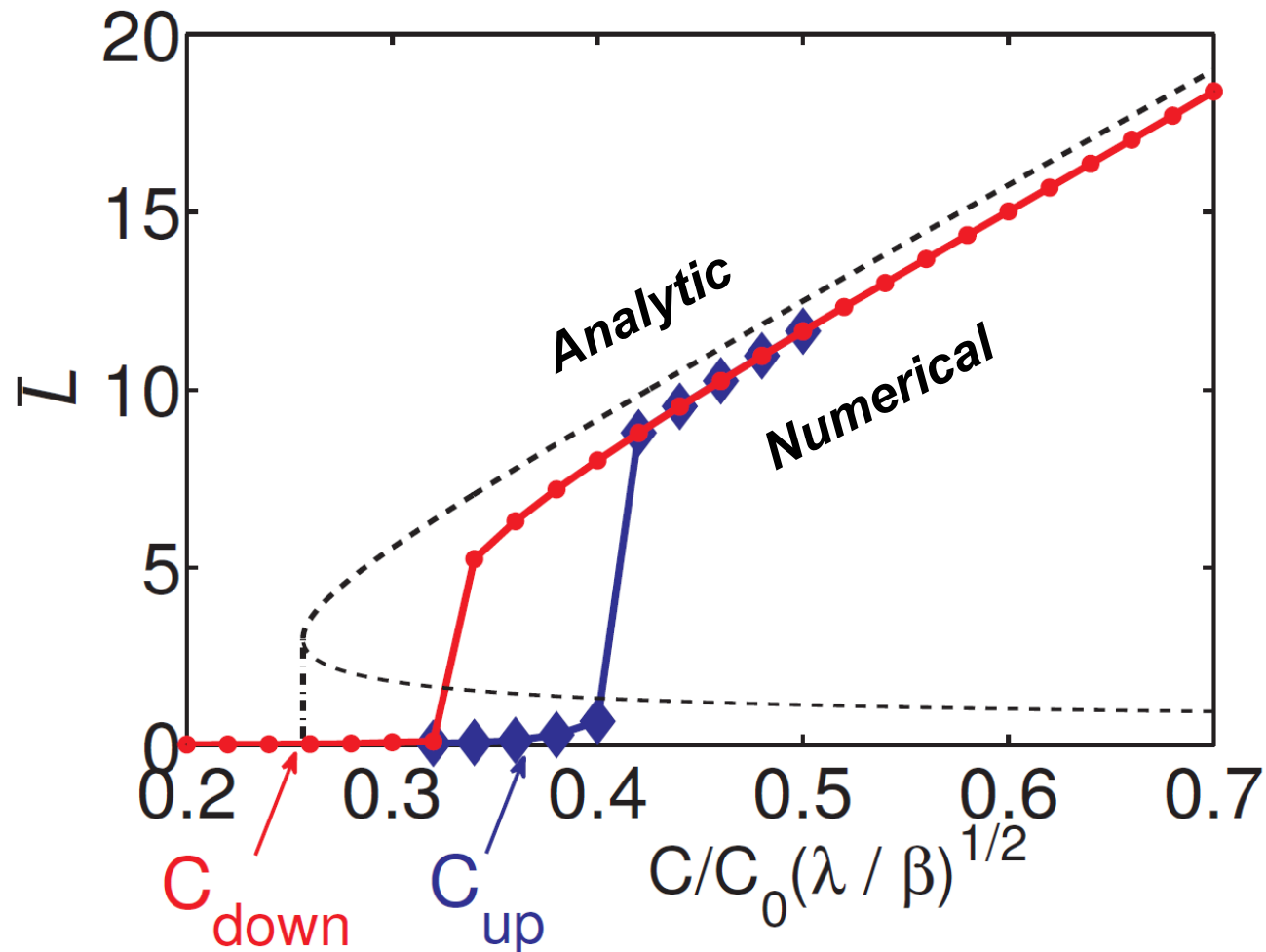
The autocatalytic pool of long chains emerges via 1st order transition:

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

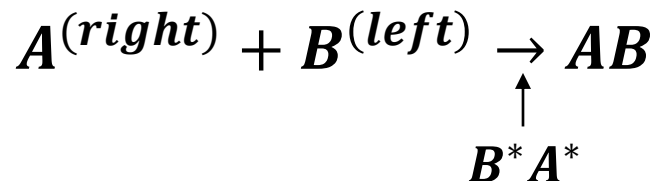
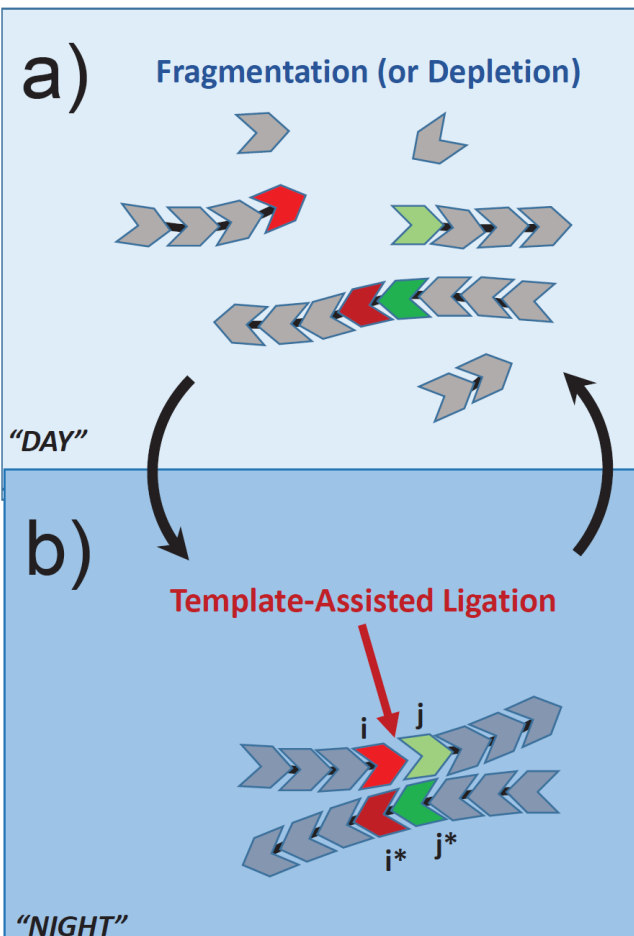
- minimal monomer concentration

First Order Transition

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



What about sequences?



Let any pair of consecutive letters ("doublet"), work as a template for ligation:

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

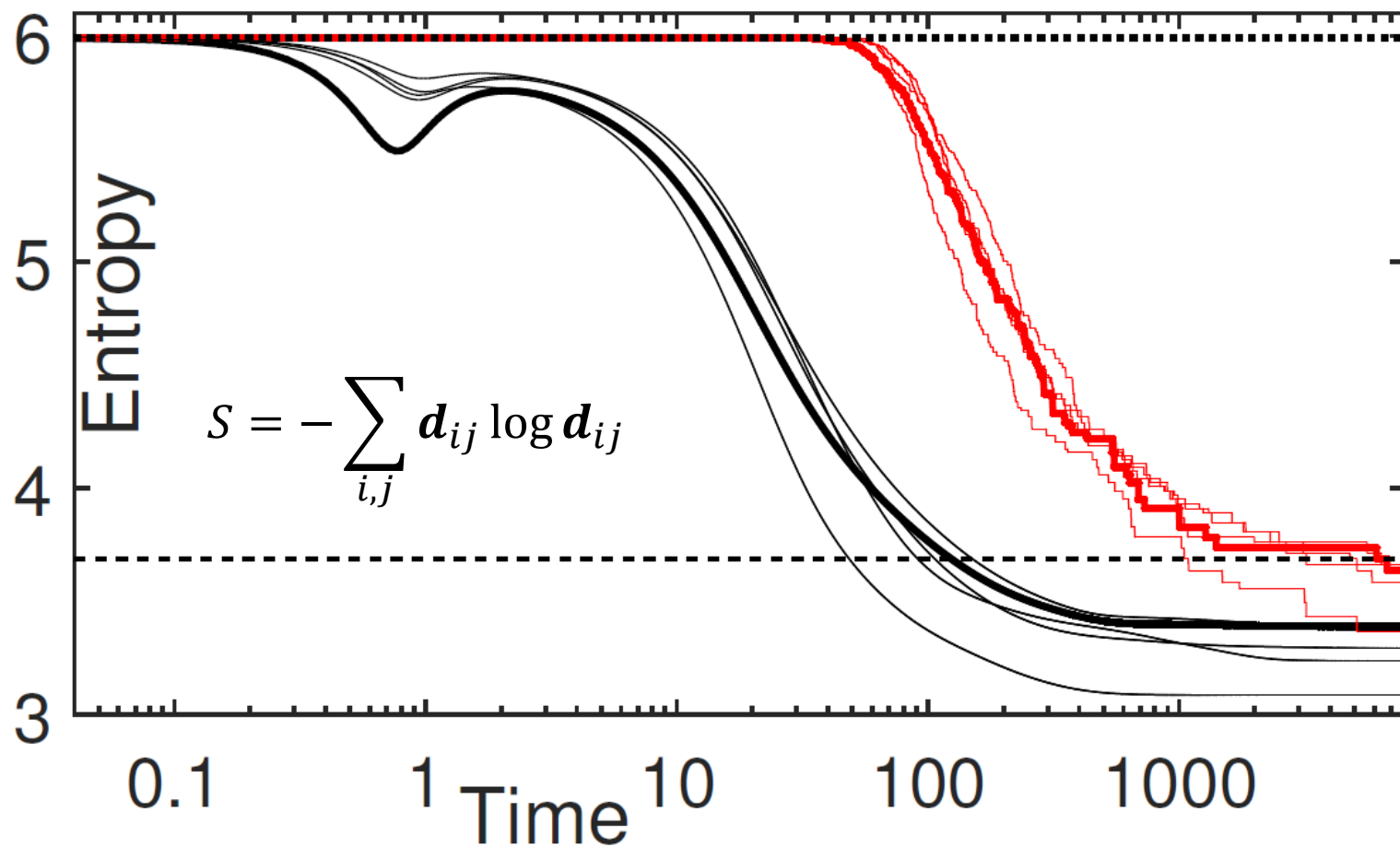
$$l_i + \sum_j d_{ij} = r_i + \sum_j d_{ji} = C_i \quad (\text{monomer conservation})$$

i^* is complementary to i ($i, j, i^*, j^* = 1 \dots Z$).

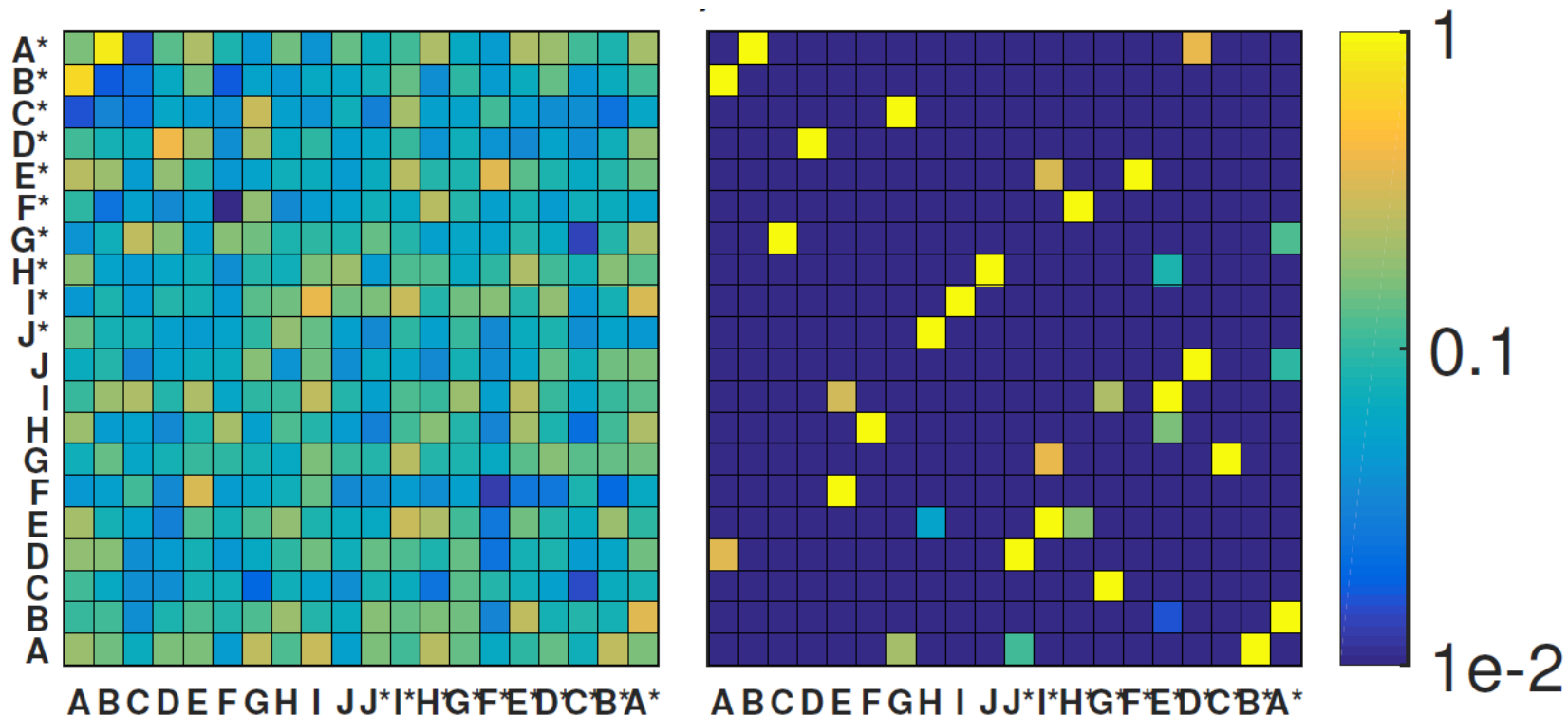
d_{ij} – density of "doublets", pairs of given consecutive letters anywhere in the pool.

l_i, r_j – density of "left" and "right" chain ends terminated with "i"
 λ_{ij} and β_{ij} are 'ligation' and 'fragmentation' rates.

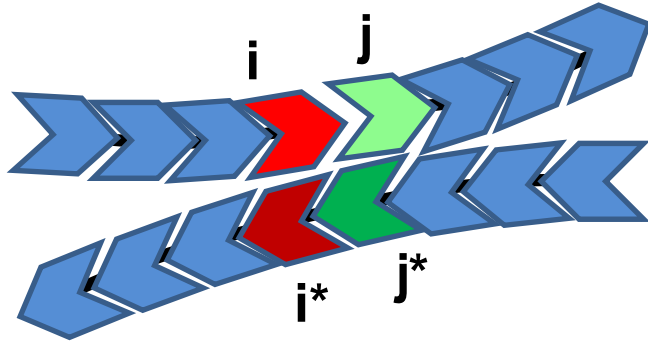
Information Entropy decreases!



Evolved “doublet” matrix



Survivor game



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

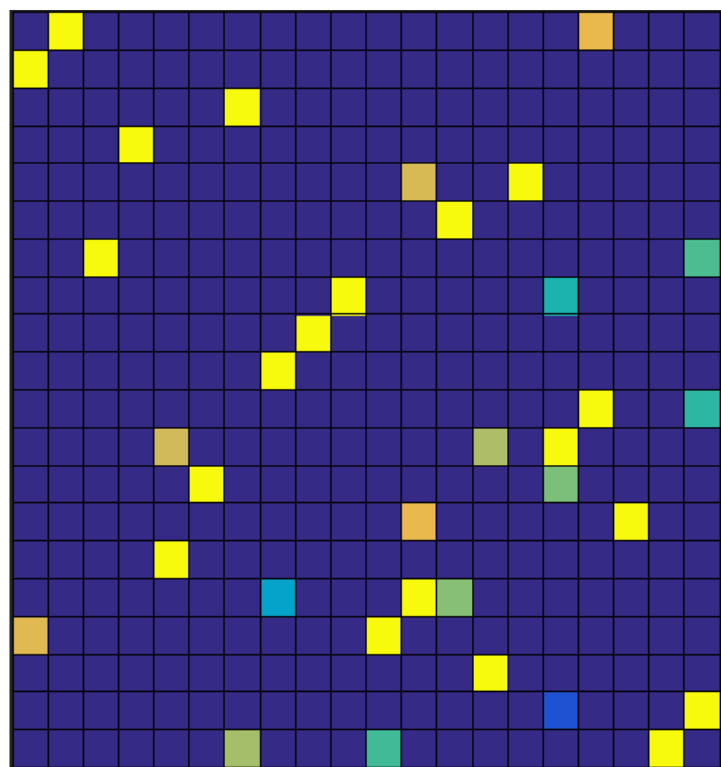
$$-\det = \lambda_{ij}\lambda_{j^*i^*}(r_i l_{i^*})(r_{j^*} l_j) - 1 \rightarrow \begin{cases} > 0: \text{growing} \\ = 0: \text{steady} \\ < 0: \text{"extinct"} \end{cases}$$

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

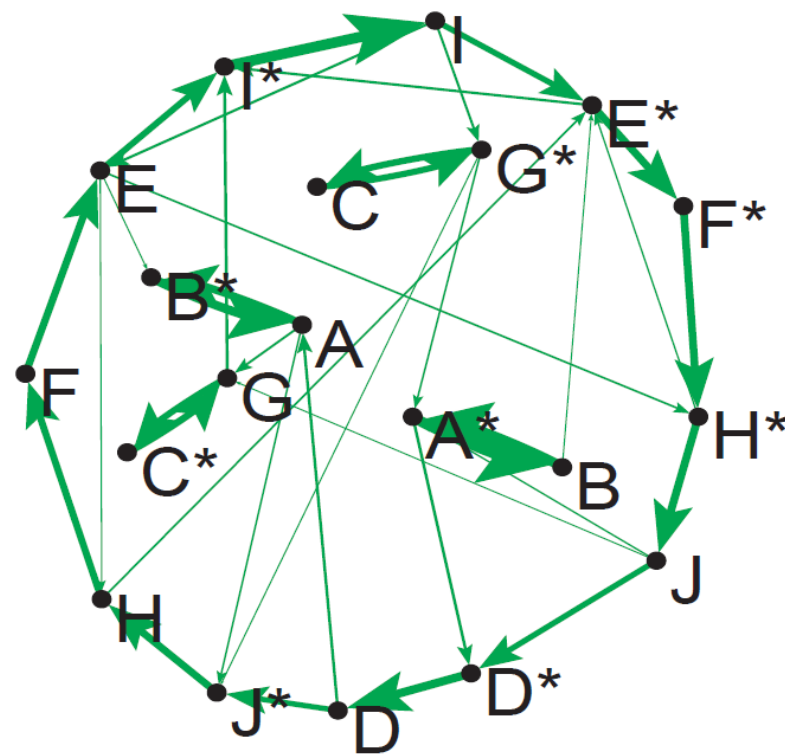


The upper bound on number of surviving doublets is **2Z**, not **Z²**

deBruin graph representation



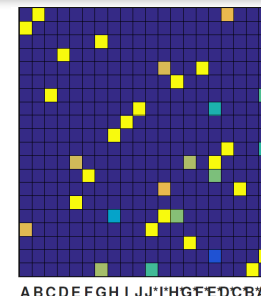
ABCDEFGHIJ J* I* H* G* F* E* D* C* B* A*



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

Searching for a “better” Life

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

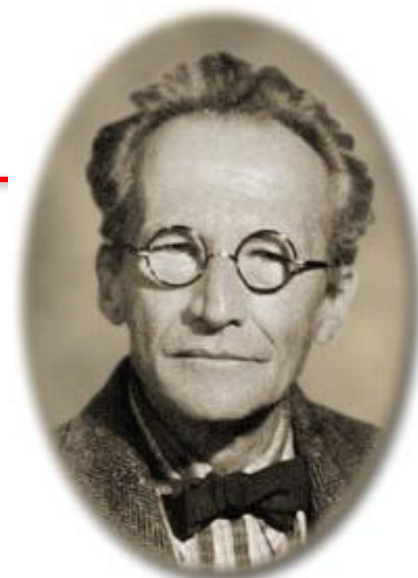


Multiple realizations of $\{C_i\}$ \rightarrow efficient sampling of the sequence space

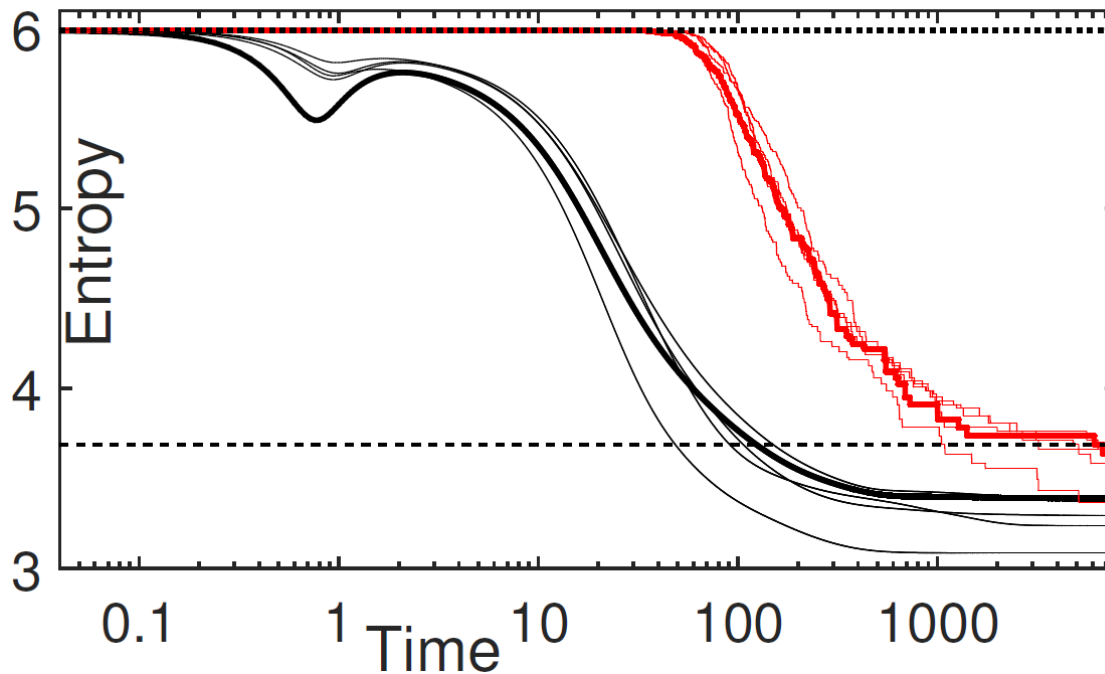
What is life?

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)



Center for Functional Nanomaterials
Brookhaven National Laboratory



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