ASTROCHEMISTRY

FROM THE BIG BANG TO LIFE

Global Astrochemistry Lecture Series (GALS) 2024

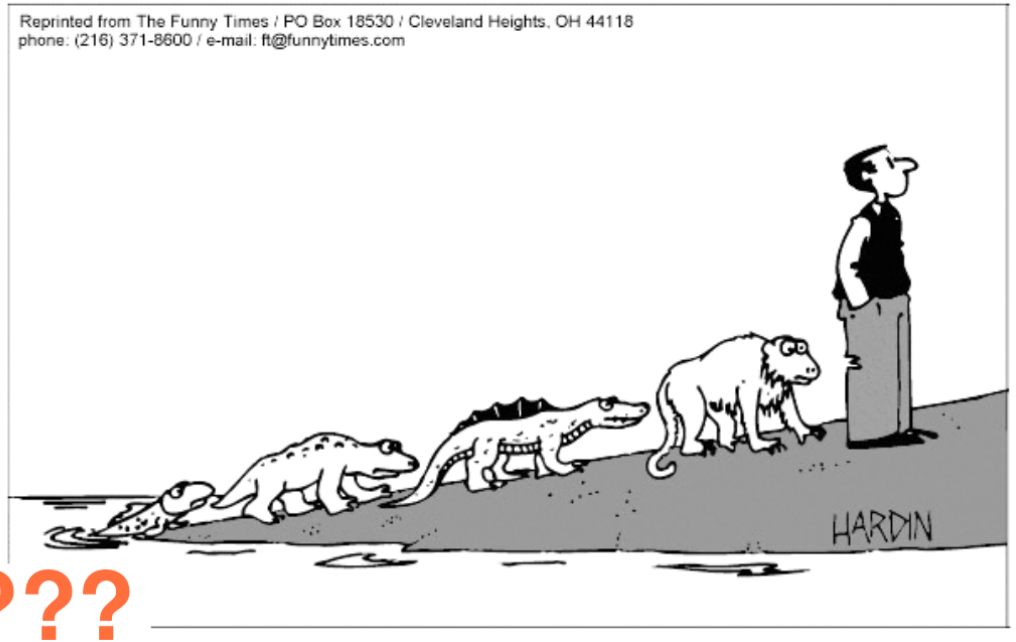
BASICS OF (BIO)CHEMISTRY

Dieter Braun. *Ludwig Maximilian University of Munich, Germany*

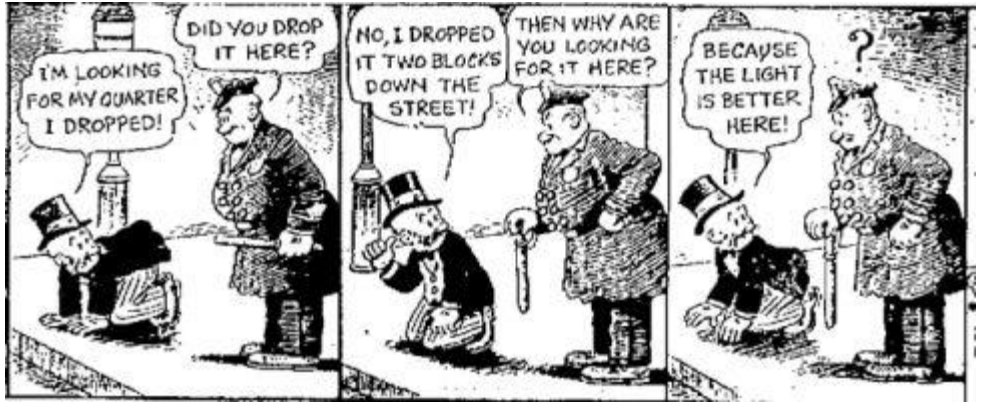
09.04.2024 | 15:00 - 17:00 CET

Origin of Life Fundamentals

How did we get here?

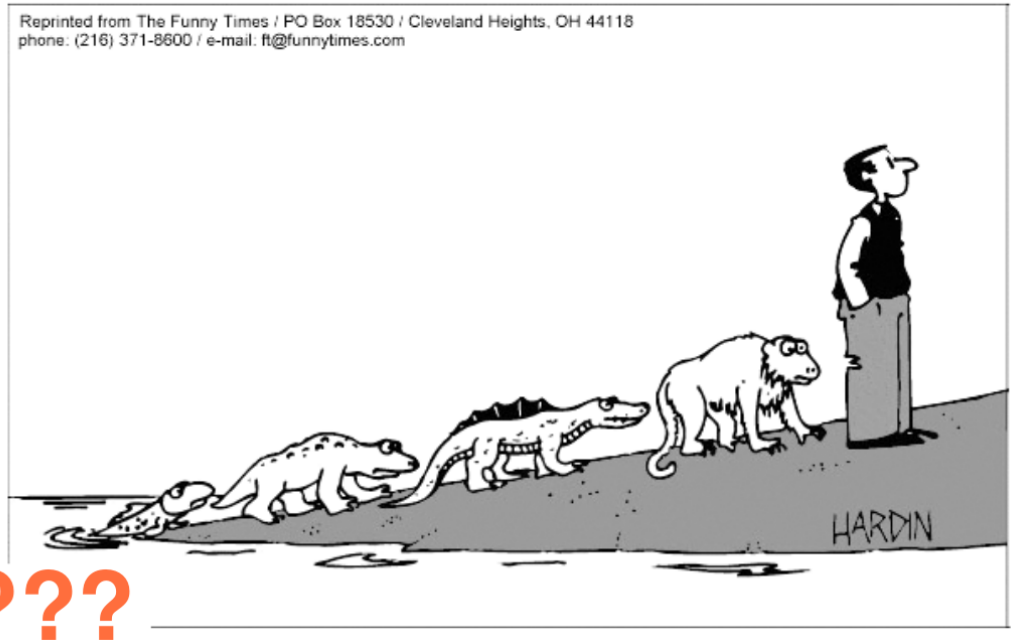


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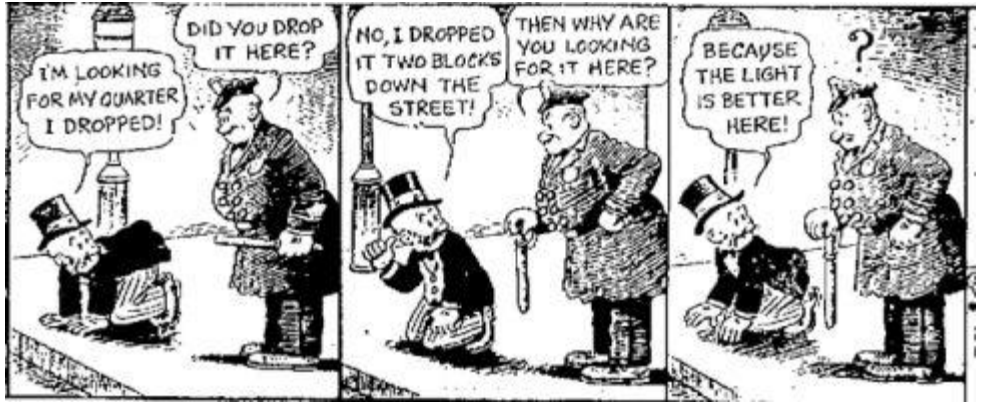


To work against powerful disciplinary reflexes in Astrophysics, Chemistry, Biology, Physics is intimidating.

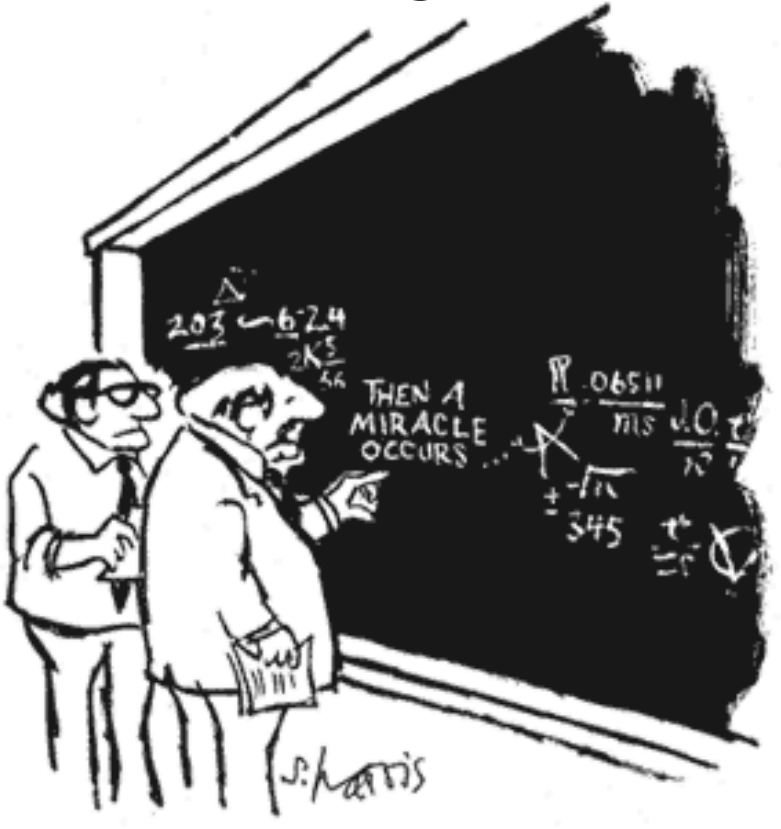
How did we get here?



???



Evolution and the Origins of Life



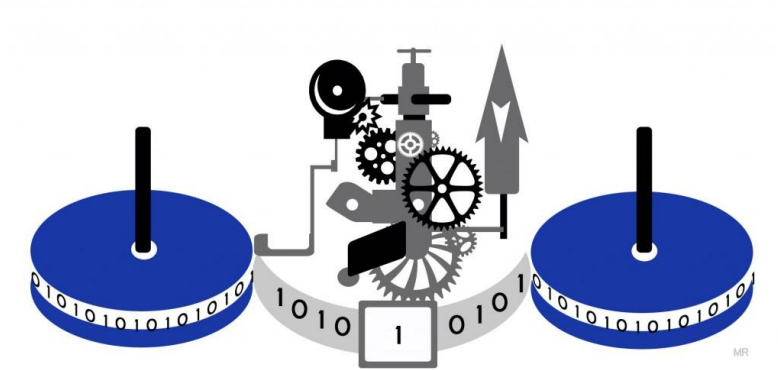
"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

What is life?

What is life?

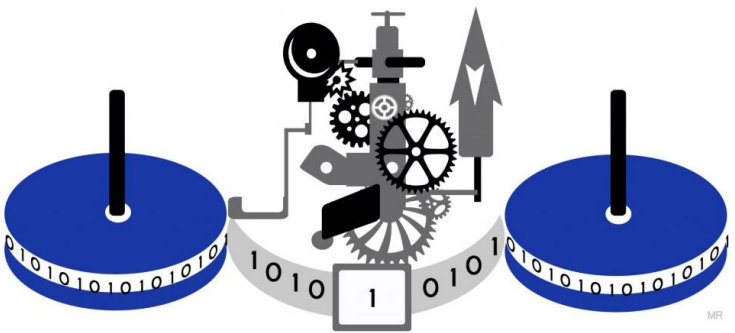
Nasa working definition of Life:
A self-sustained chemical system
capable of undergoing Darwinian Evolution

Logic of Molecular Biology

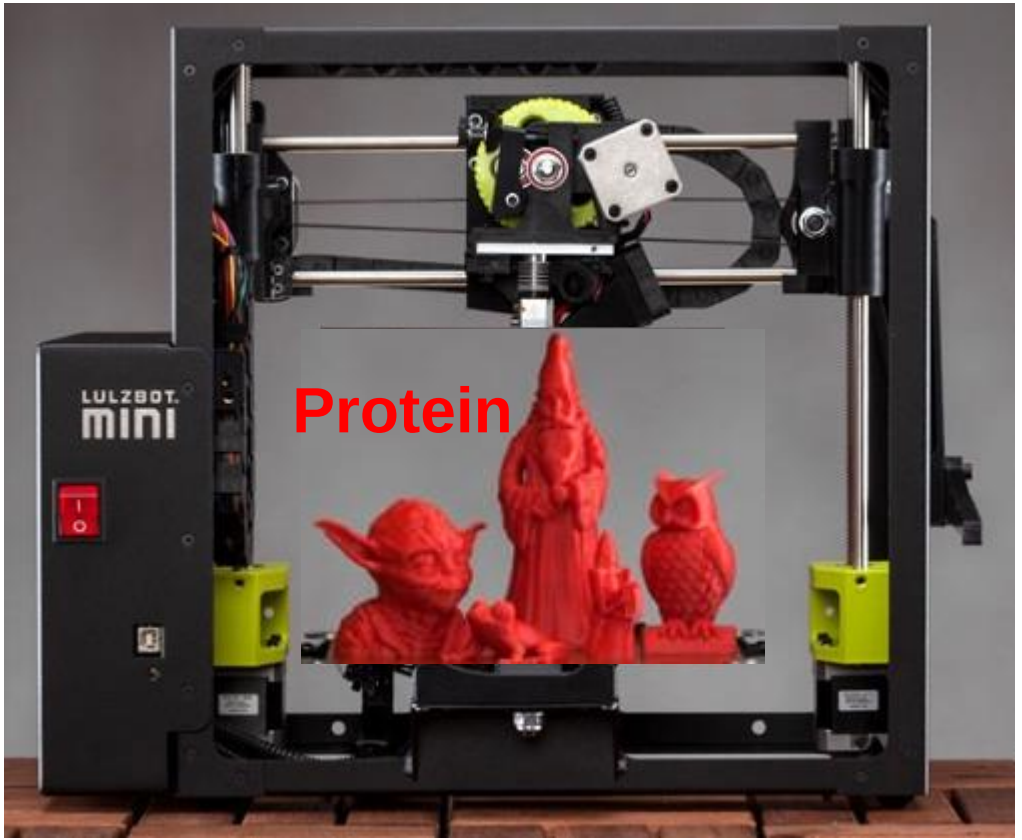


Storage of information very similar to Turing machine => Computer

Logic of Molecular Biology

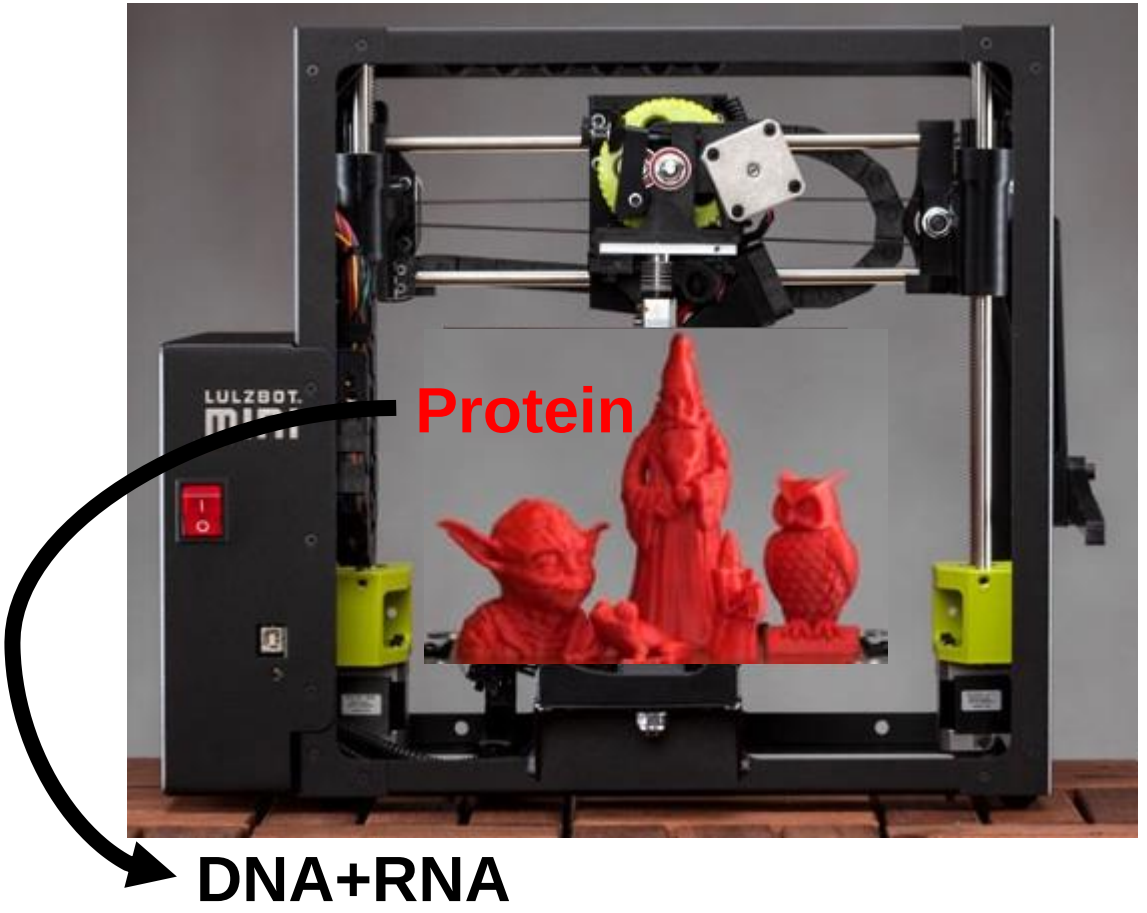


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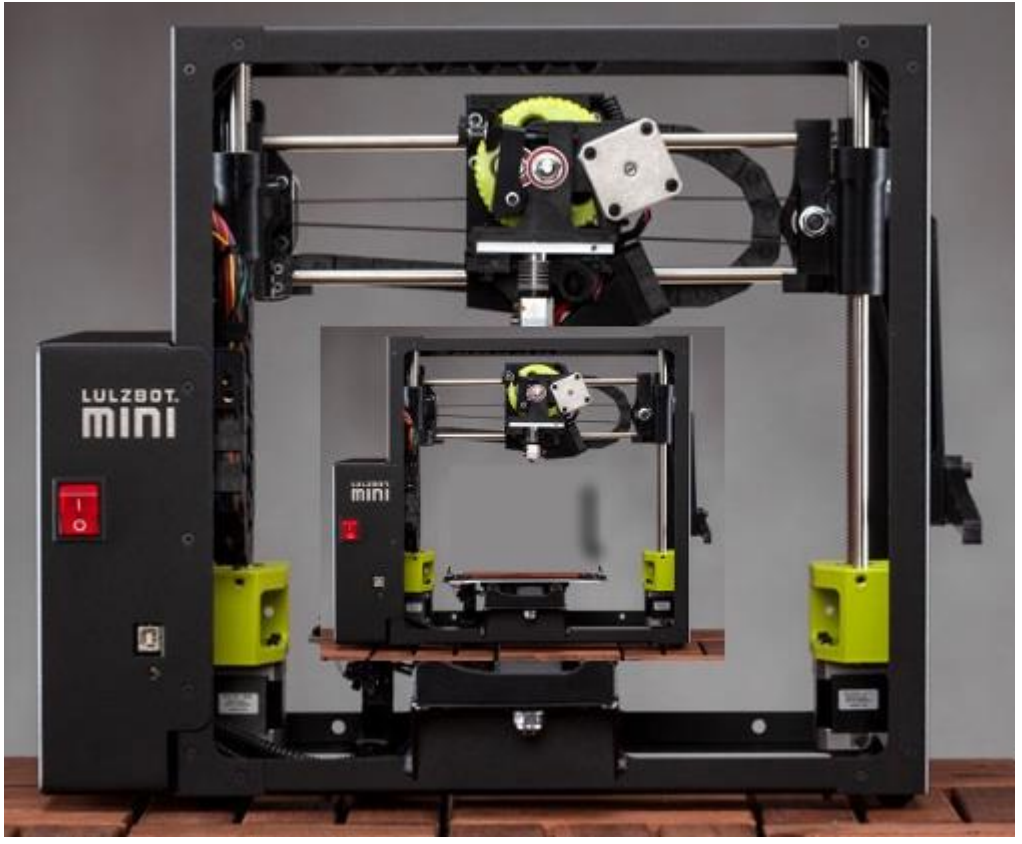
DNA+RNA

Logic of Molecular Biology

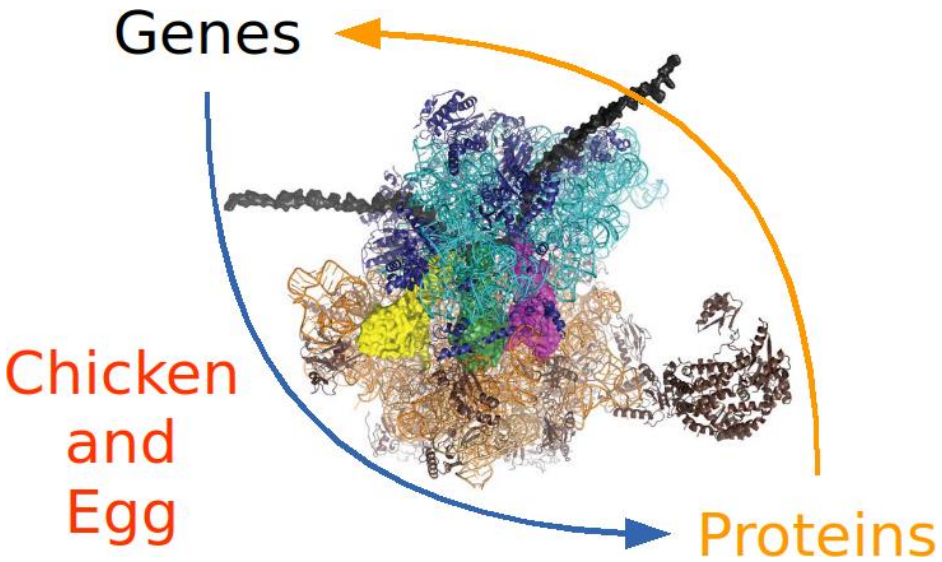


Logic of Molecular Biology

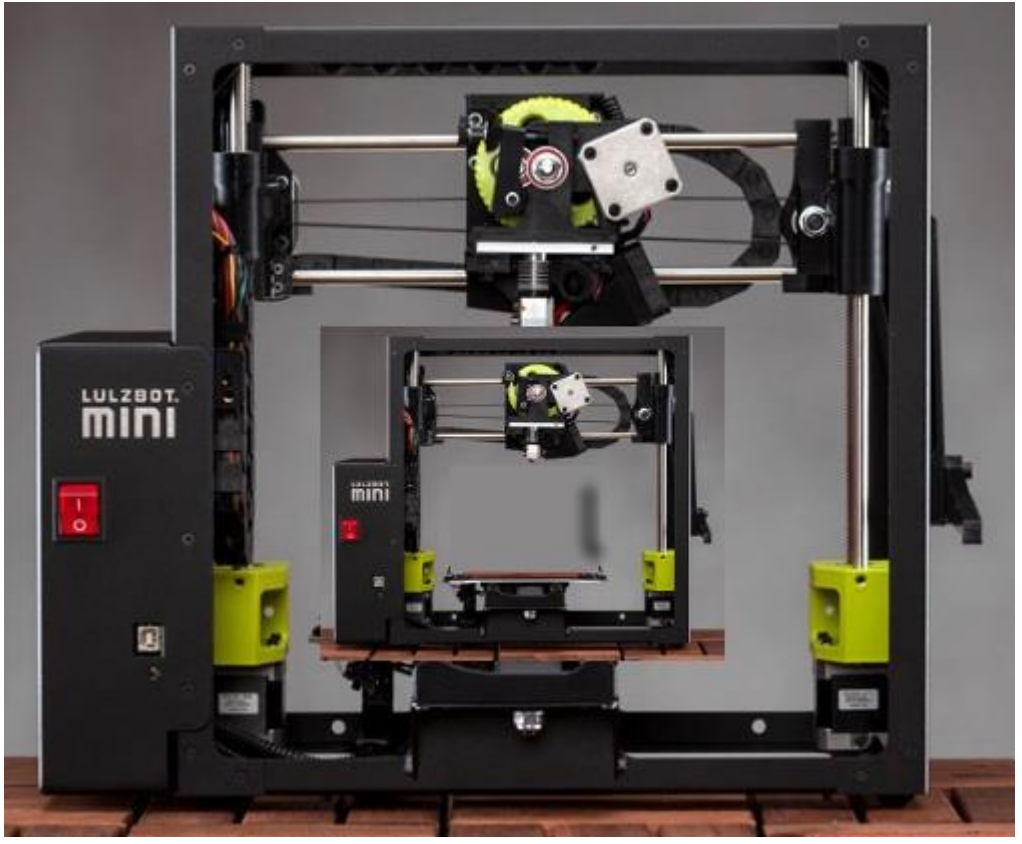
How to make a machine that makes itself?



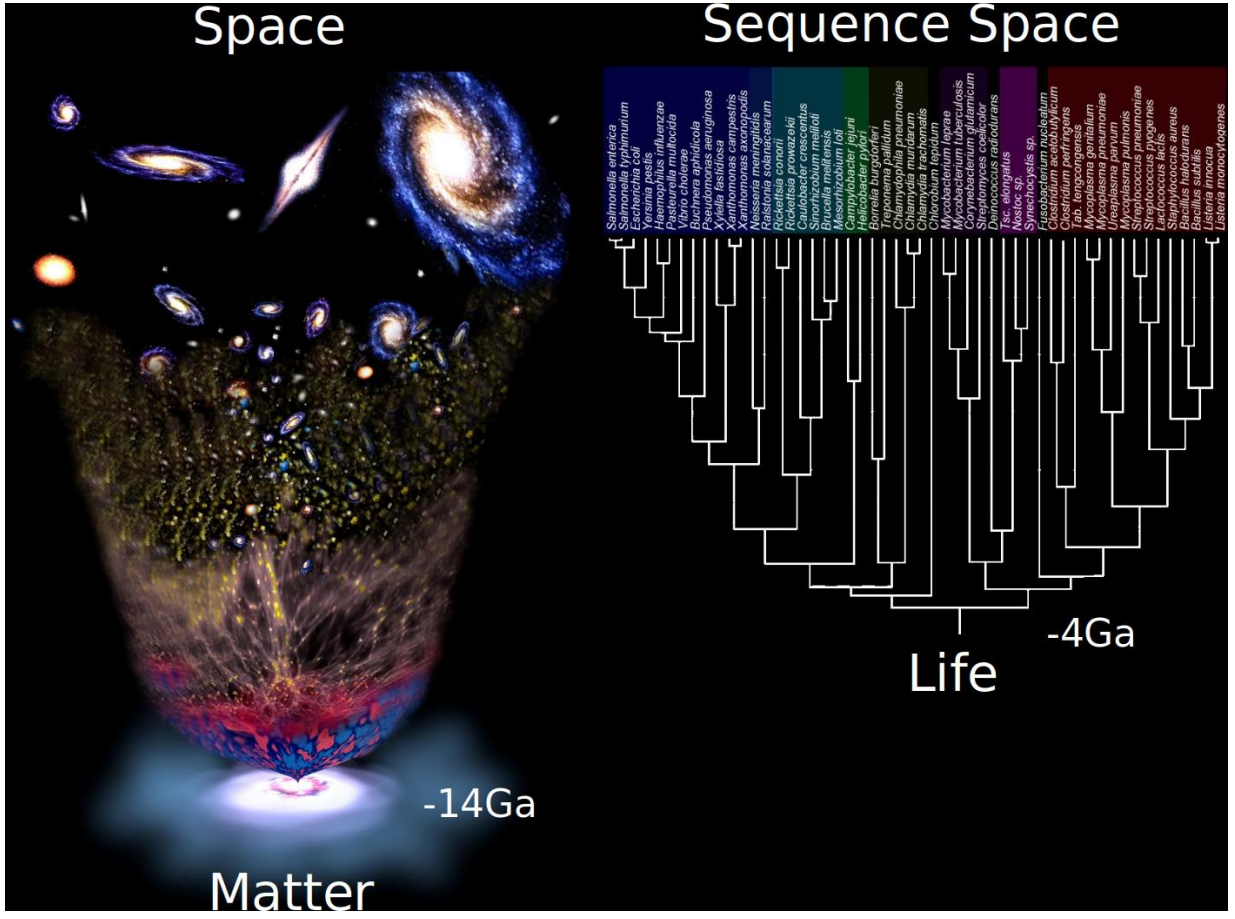
Logic of Molecular Biology



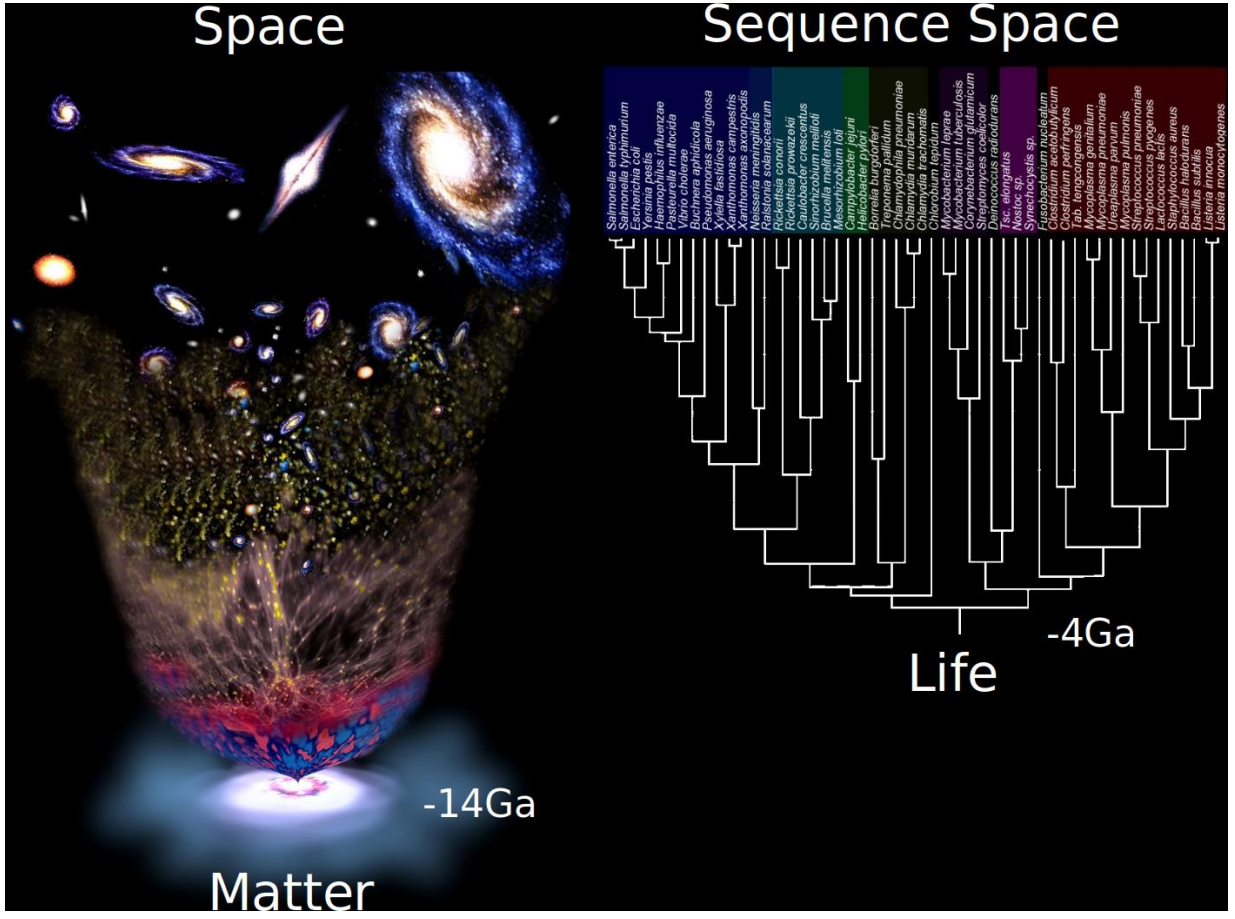
How to make a machine that makes itself?

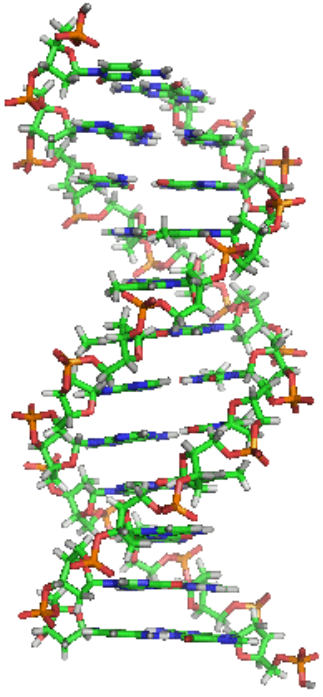


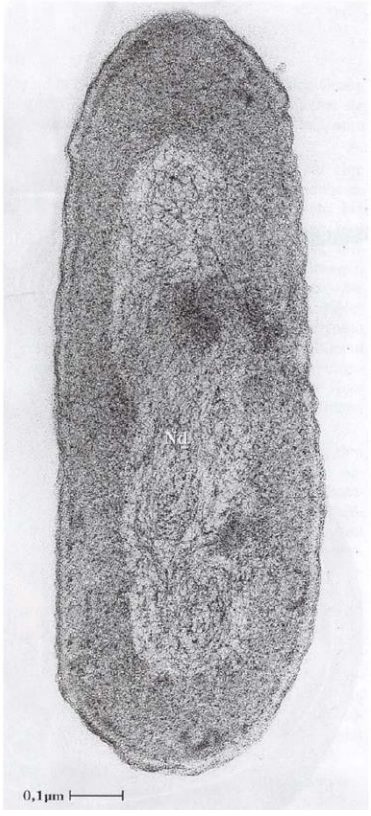
History of Biology



History of Biology

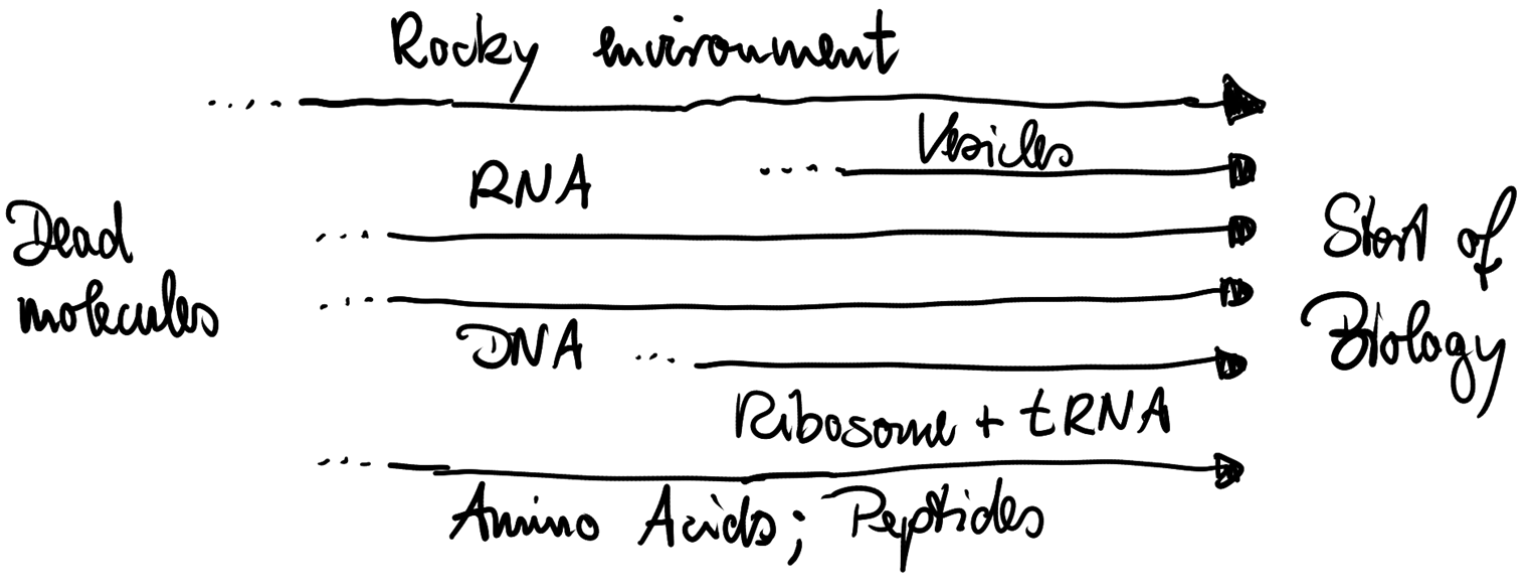






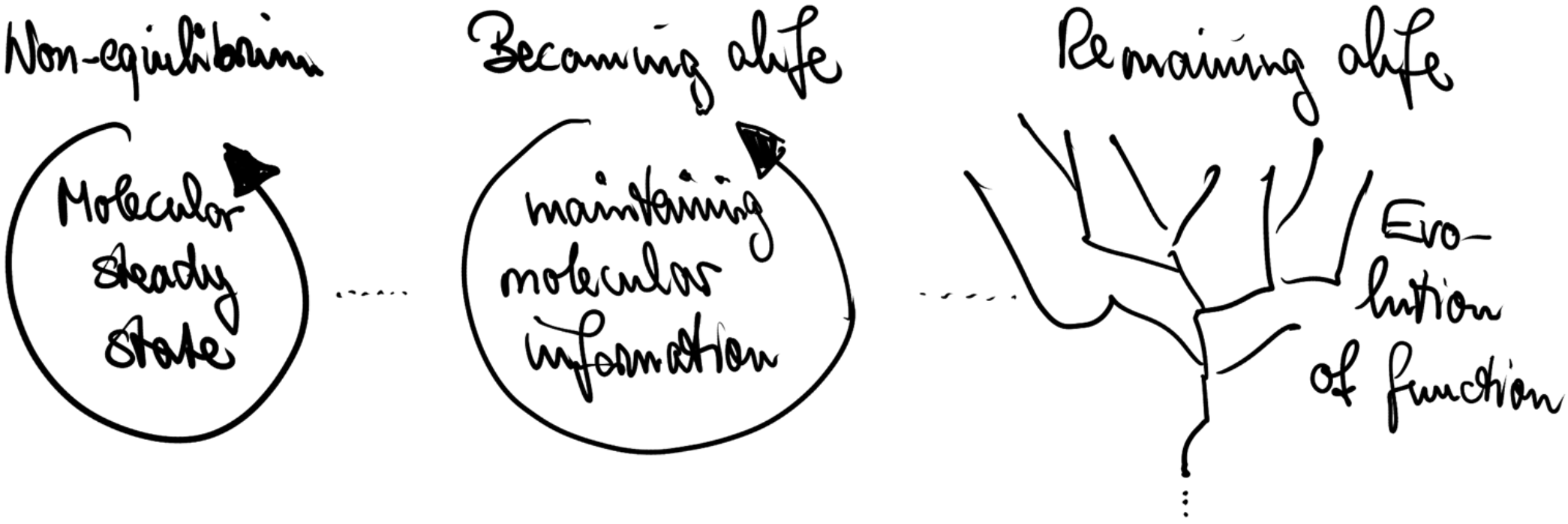
History of Biology

History of Biology

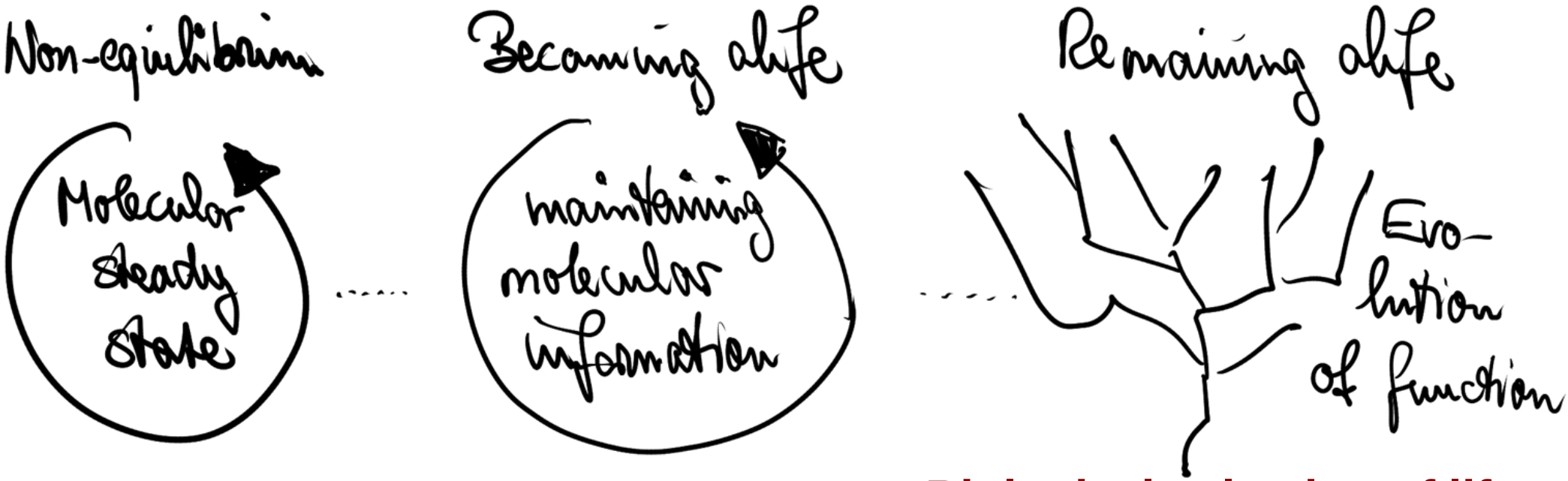


Becoming alive

Becoming alive



Selection before and within life

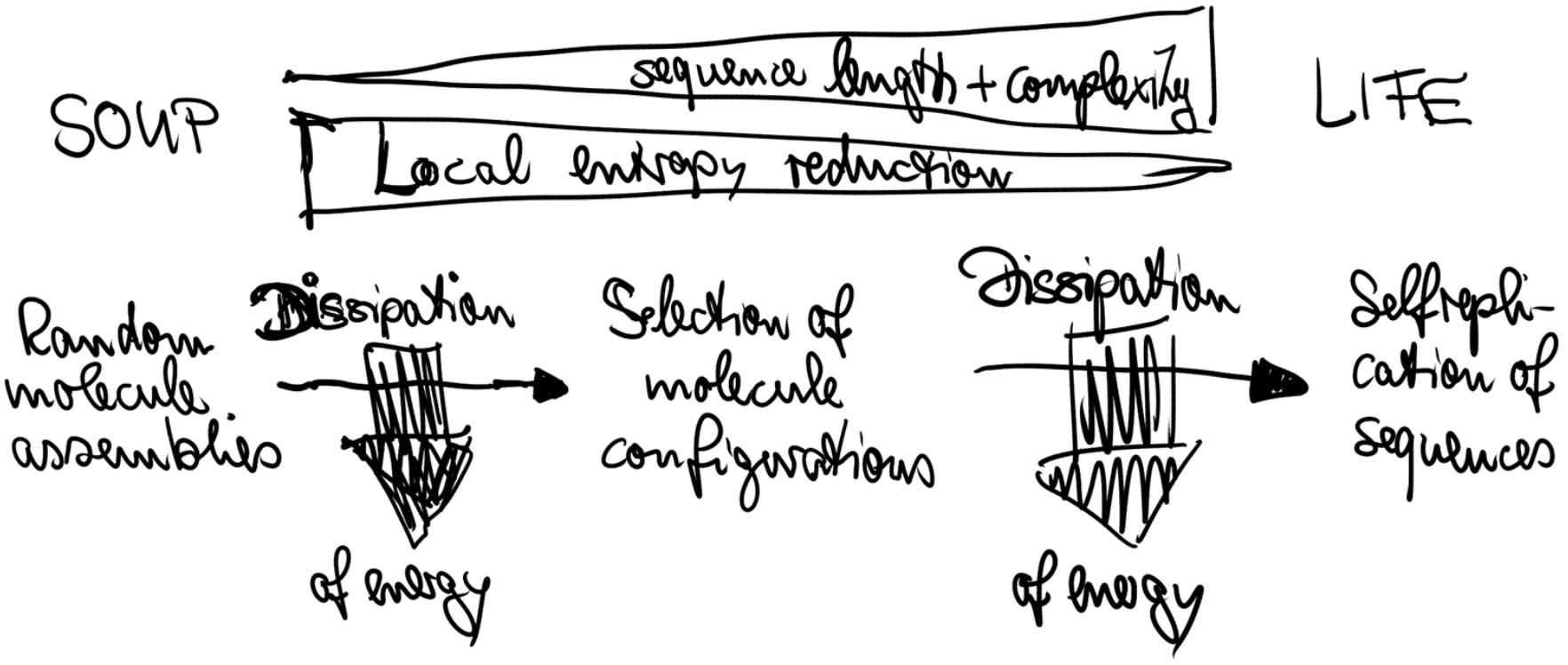


Physical selection from non-equilibrium boundary conditions

Biological selection of life against other life to adapt better to environments

Soup of life

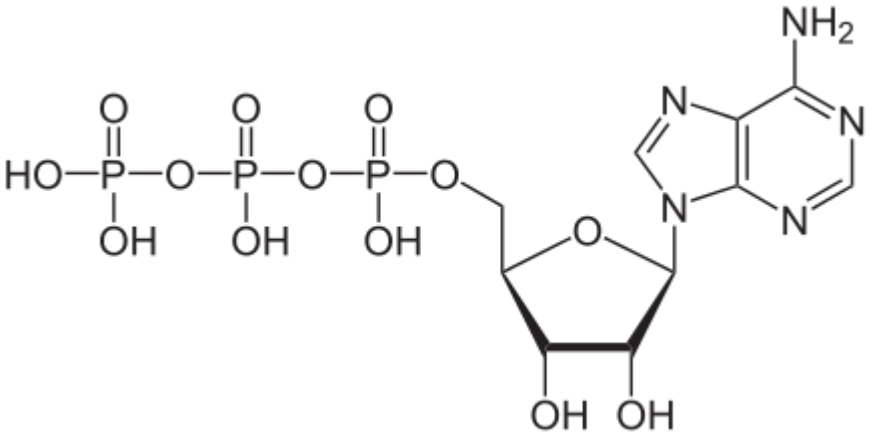
Soup of life


SOUP
sequence length + complexity
LIFE
Local entropy reduction
Random molecule assemblies
Dissipation
of energy
Selection of molecule configurations
Dissipation
of energy
Self-replication of sequences

Three faces of entropy:

1. Activation of Molecules to drive reactions.

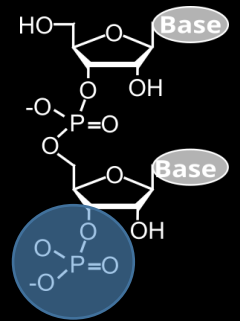
From biology: misleading leaving groups



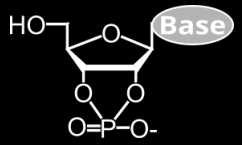
Molecular Entropy: ATP vs AMP, activation, nucleophiles, leaving group

Polymerization and hydrolysis of RNA

Make RNA



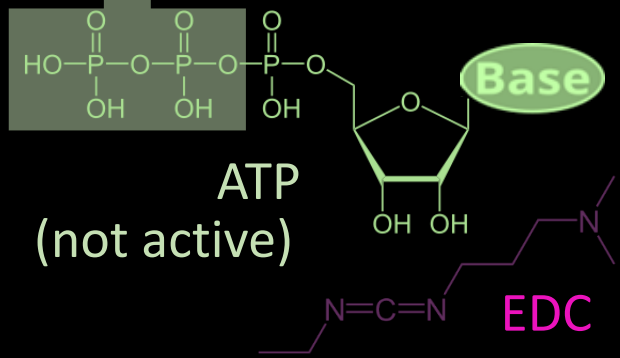
- H_2O



Leaving group

Waste

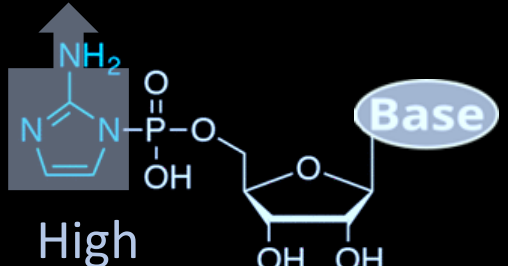
Biology



ATP
(not active)

EDC

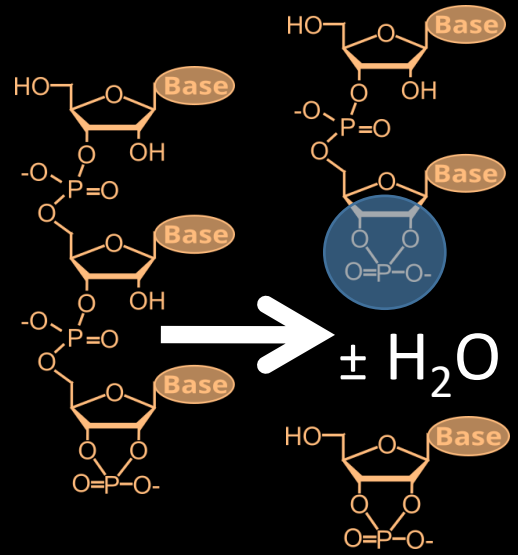
Waste



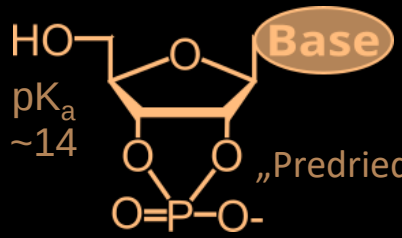
High
$MgCl_2$

Strand separation?
Recycling? Activation?

Break RNA

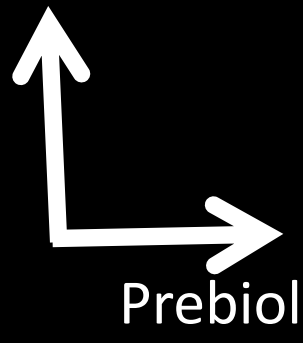


Ring opening ligation



Findings:
- pH 9-11 sufficient
- No divalent ions
  (strands separable)

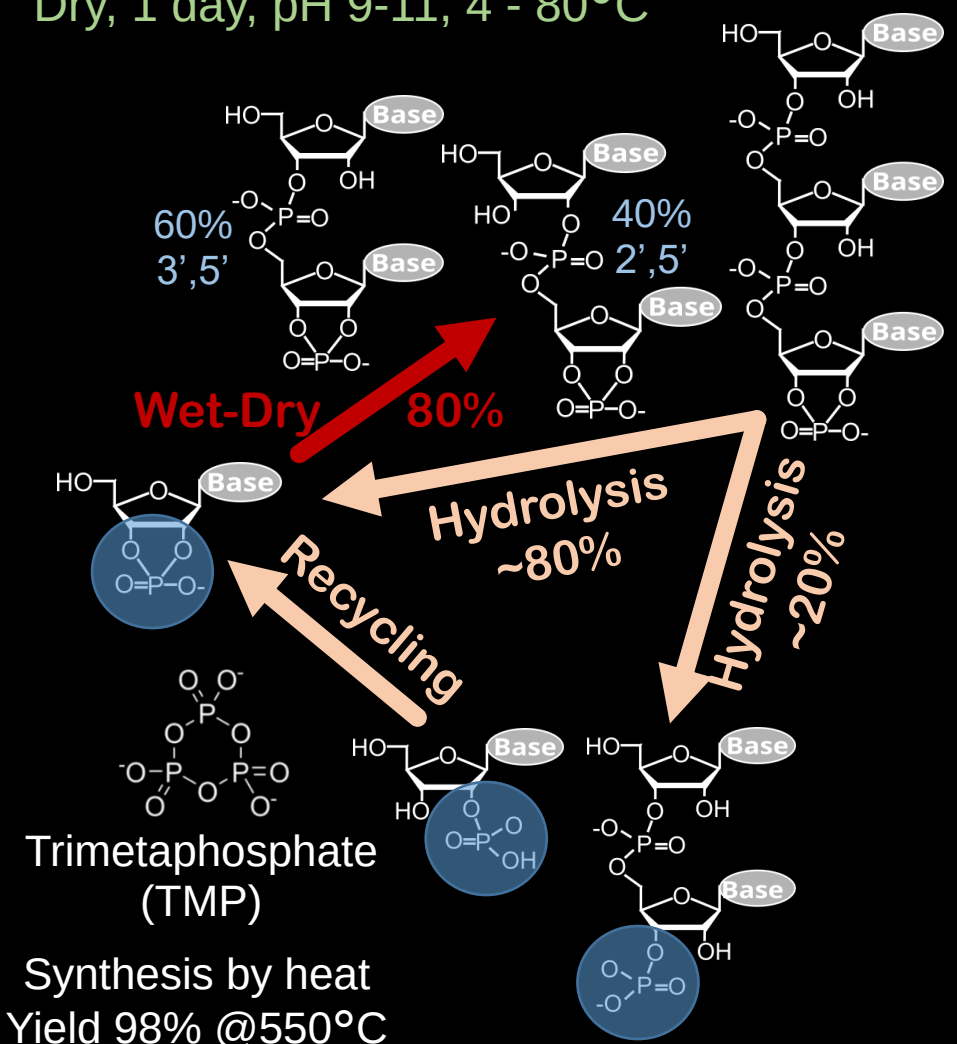
- Only shuffle around H_2O
- Minimal side products
- RNA bases G+U buffer at 9-10
- 70% polymerization yield
  (with Tommaso Fraccia, Milano)



Chemical Evolution

RNA oligomerization in “dry” state

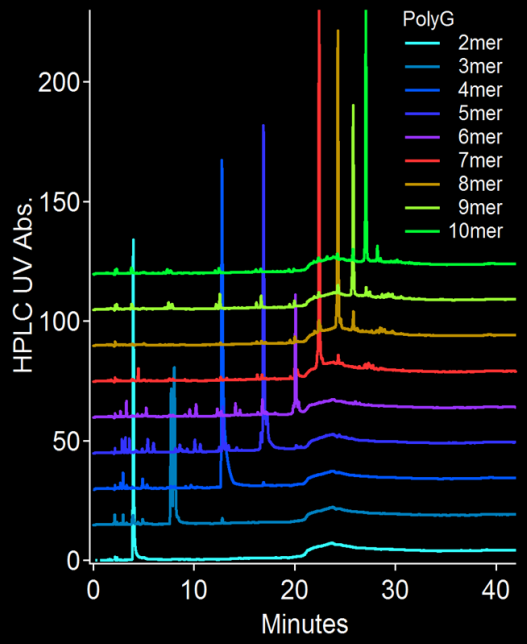
Dry, 1 day, pH 9-11, 4 - 80°C



Trimetaphosphate (TMP)

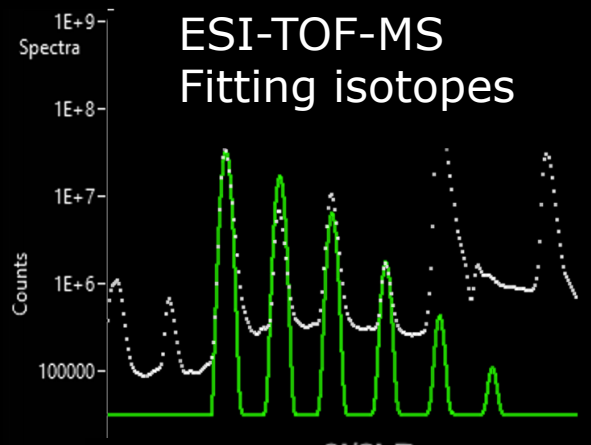
Synthesis by heat
Yield 98% @550°C

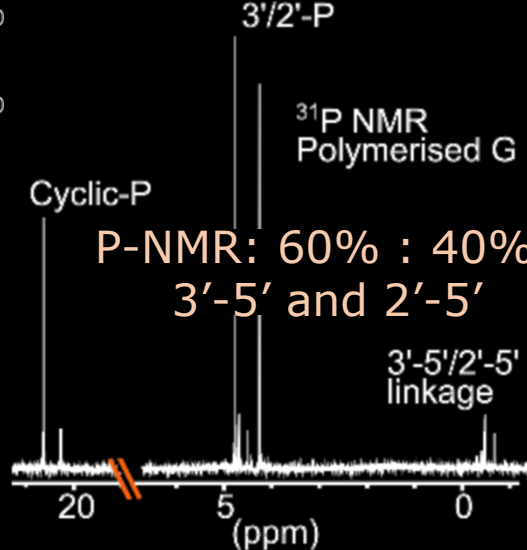
HPLC @ 60°C



ChemSystemsChem
doi.org/10.1002/syst.
202200026 (2022)

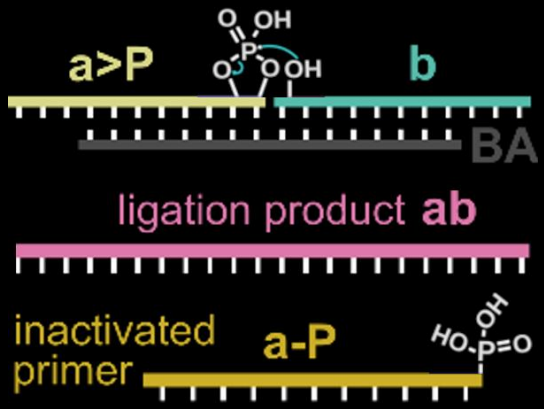
ESI-TOF-MS
Fitting isotopes

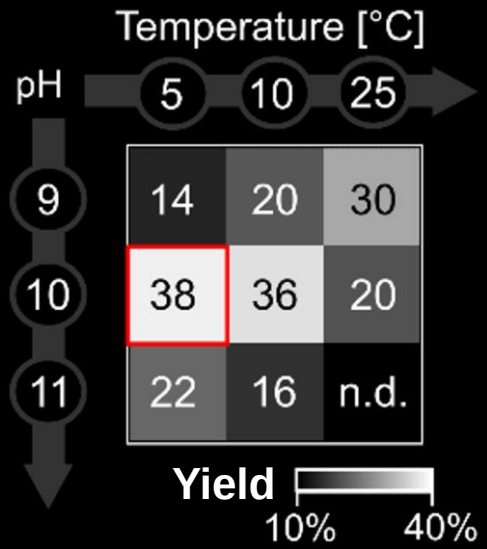


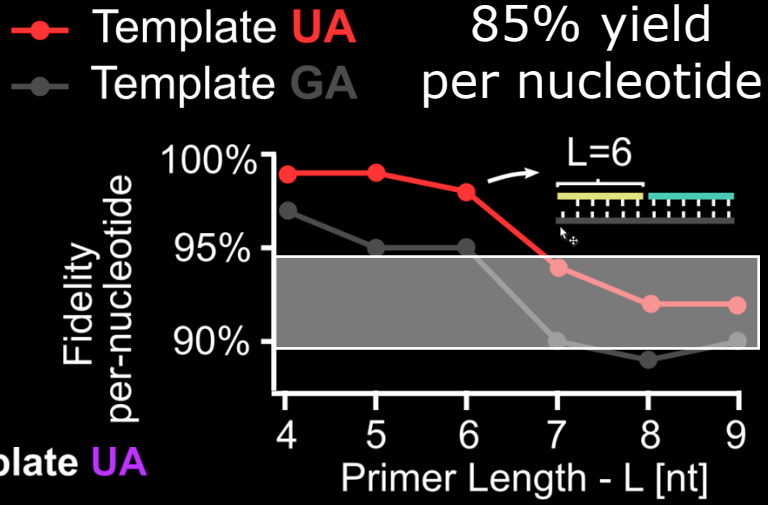


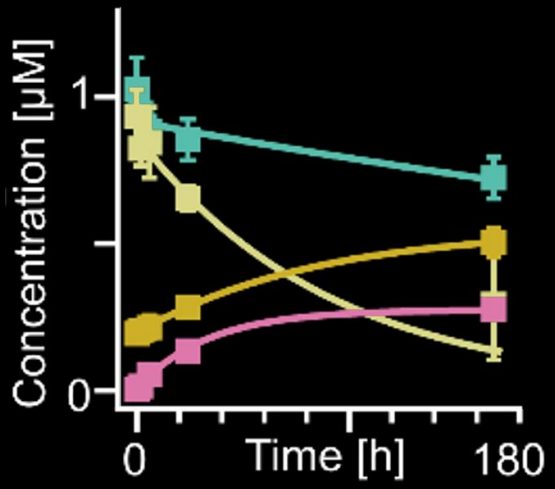
P-NMR: 60% : 40%
3’-5’ and 2’-5’

Templated ligation of RNA at low Mg^{2+} concentration

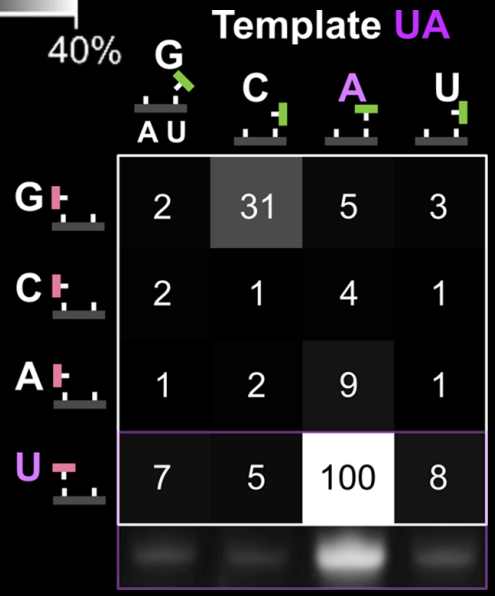


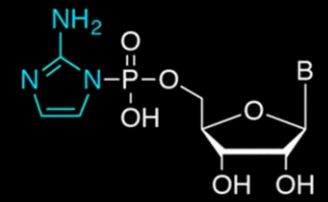






[a],[b],[ba] = 1µM 50mM CHES
1mM $MgCl_2$ pH 10, 10°C

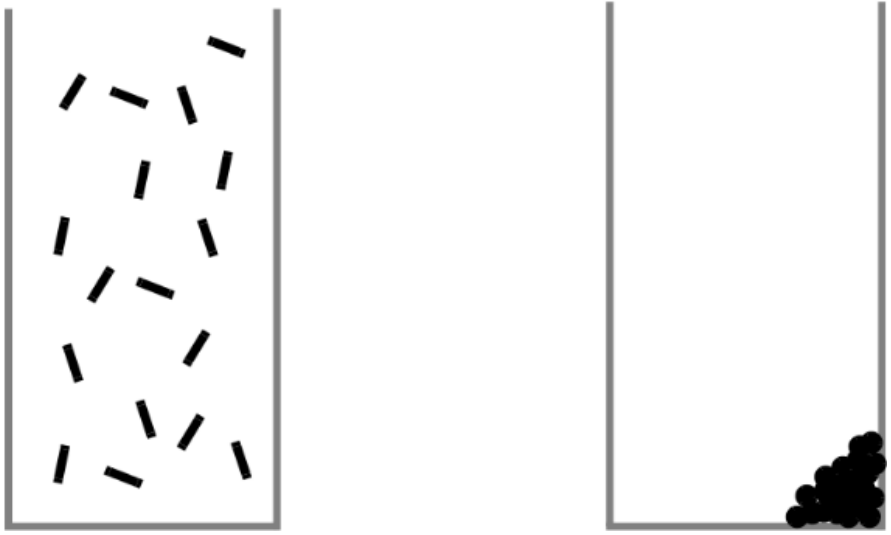




Jack Szostak et.al.

JACS
doi.org/10.1021/jacs.3c10813 (2024)

Three faces of entropy:
2. Enhancing the chemical potential (accumulation)



Nota bene:
- Vesicles do not accumulate
- Coacervate do not enhance chemical potential

Localization Entropy: chances to find molecules, probability of reaction, leaving group

Three faces of entropy:
3. Informational sequence entropy

$$H(X) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

ATTTTTATATATAAAATATATATA

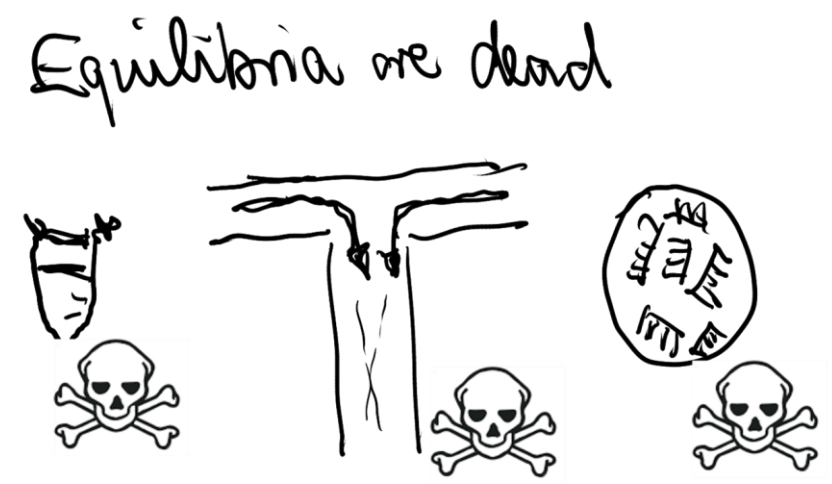
Sequence Entropy: information stored in DNA or RNA to be replicated

Death of equilibrium



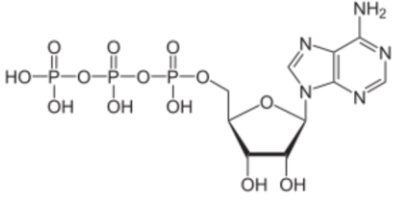
Death of equilibrium

Death of equilibrium



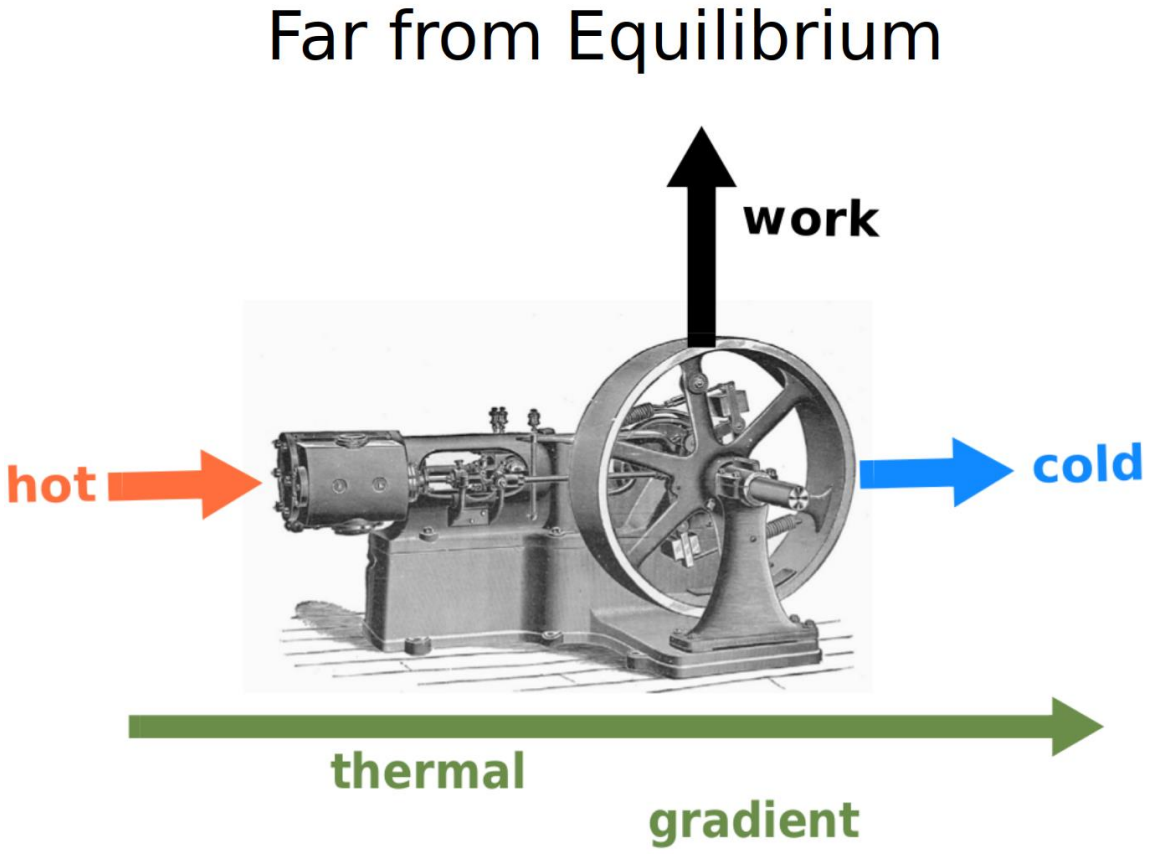
Assumed nonequilibrium



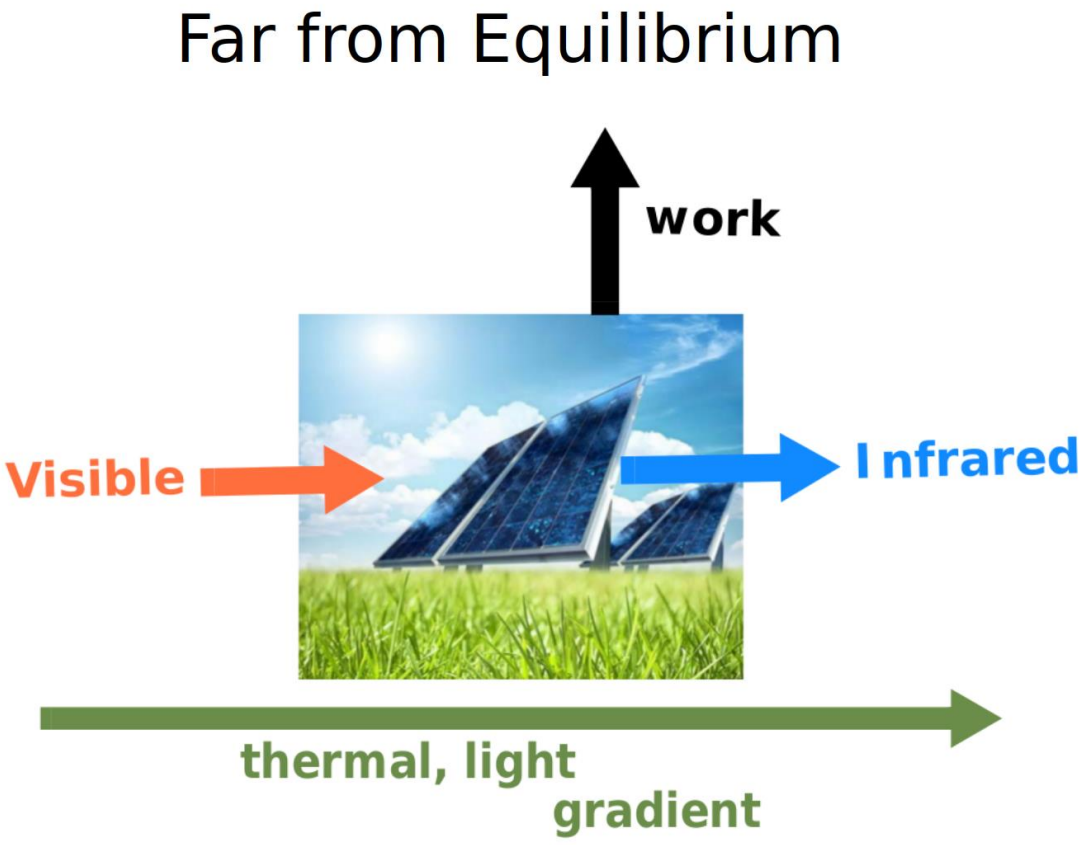


Modes of non-equilibrium

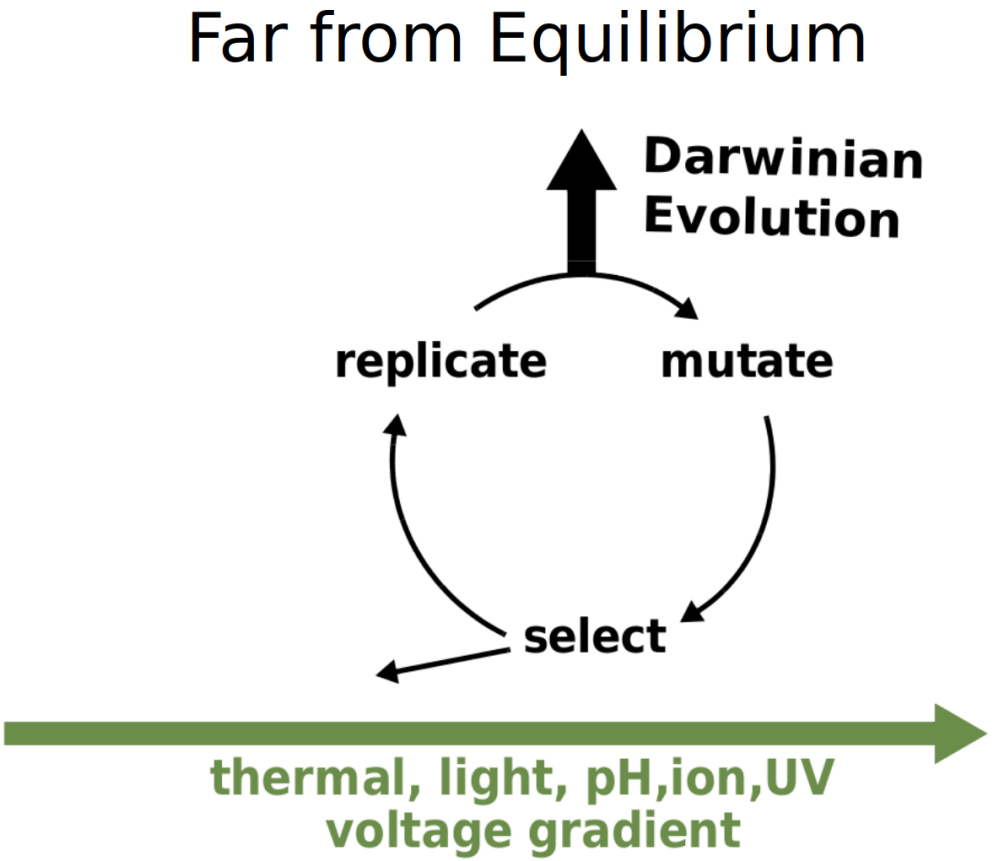
Modes of non-equilibrium



Modes of non-equilibrium

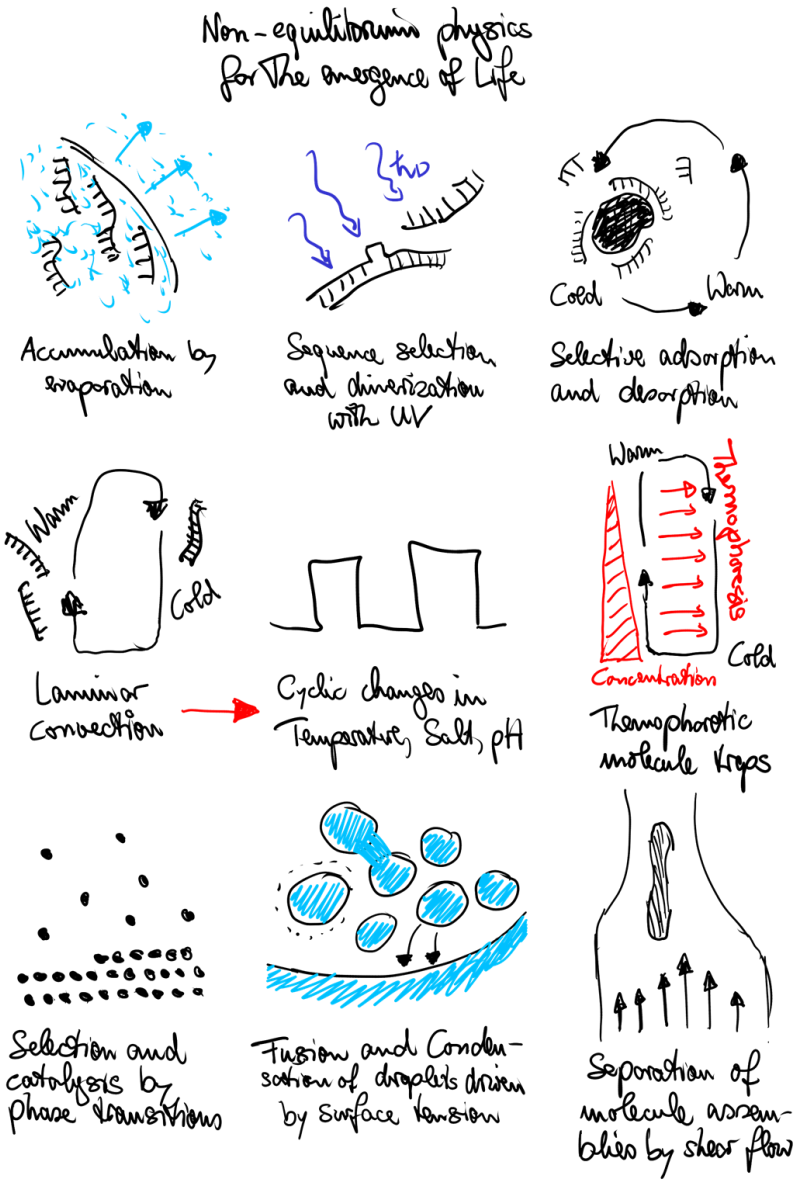


Modes of non-equilibrium



Modes of non-equilibrium

Modes of non-equilibrium



Structure of Origin of Life

Nucleotides (possibly stored)

Chemical conditions:
- Polymerization
- Ligation
- Activation

Physical non-equilibrium:
- Strand separation
- Maintaining accumulation
- Feeding and
  Waste removal

Some upcoming molecular machines

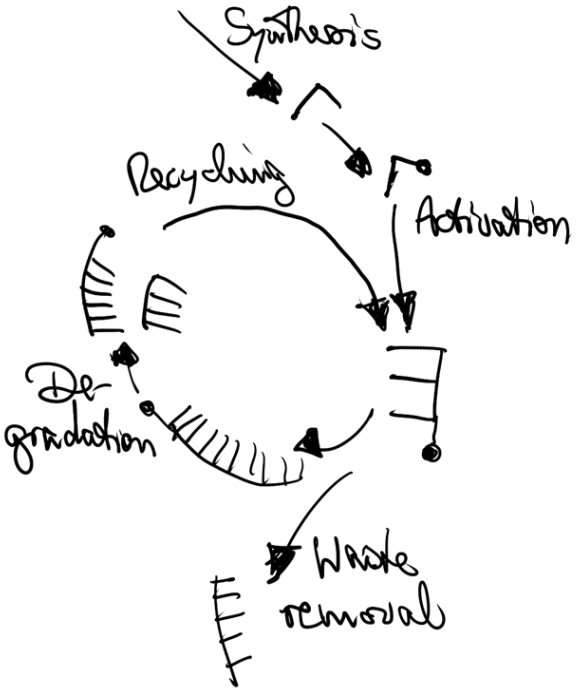
Structure of Origin of Life

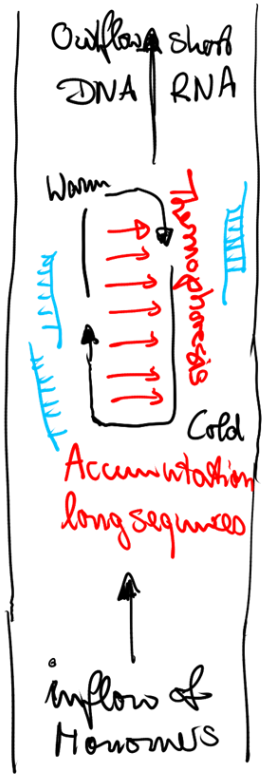
Chemical nonequilibrium in physical nonequilibrium

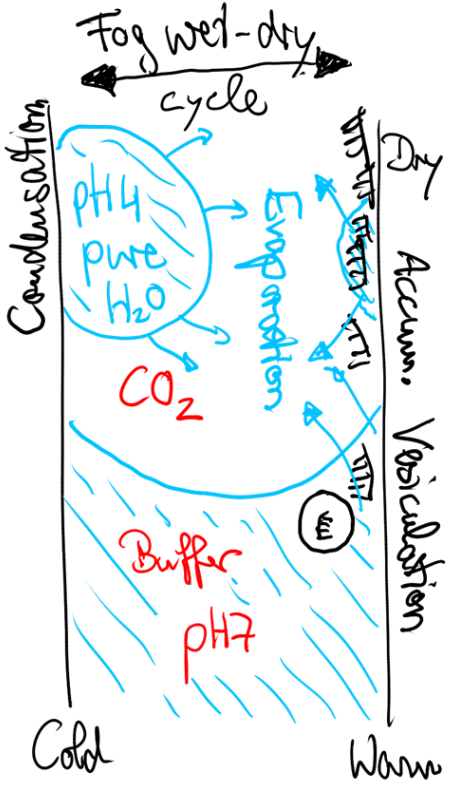
Nucleotides (possibly stored)

Chemical conditions:
- Polymerization
- Ligation
- Activation

Physical non-equilibrium:
- Strand separation
- Maintaining accumulation
- Feeding and
  Waste removal







Some upcoming molecular machines

RNA evolution in volcanic wet-dry settings

Biological Evolution

Darwinian Evolution

Strand Separation

Replication

Sequence Selection

Recycling

Inflow

Bacteria

Air

Accumulated RNA

Water

1mm

80% yield

40% yield

a>P

b

Replication by Ligation

Genet

Ribosom

NA

Cold

Warm

H_2O pH4

Dry

Wet

63mer ssDNA

Salt oscillation

DOPC

Time