INTERNSHIP PROPOSAL

Laboratory name : Gulliver Supervisor : Olivier Rivoire e-mail : <u>olivier.rivoire@espci.fr</u> Web page : <u>http://statbio.net/</u> Internship location : ESPCI, 10 rue Vauquelin, 75005 Paris

Physics models for the origins of Darwinian evolution

Life is understood to be both the result and the engine of Darwinian evolution. Darwinian evolution, also known as evolution by natural selection, occurs when three key ingredients are present: (1) Variation: a population of individuals exhibits different traits. (2) Inheritance: these individuals reproduce and pass on their traits, at least in part, to their offspring. (3) Differential reproduction: some traits lead to greater survival and reproductive success than others. When these conditions are present, natural selection can occur, leading to changes in the population over time.

In modern life forms, the mechanisms underlying variation, inheritance, and differential reproduction are complex and themselves the products of billions of years of Darwinian evolution. At the origin of life, however, Darwinian evolution must have emerged from simpler processes. What were these processes? We approach this question from a physics perspective, aiming to identify fundamental physical and chemical processes that could potentially give rise to Darwinian-like evolutionary dynamics beyond the specific pathway that led to life on Earth. [1].

To this end, we develop and analyze statistical physics models that incorporate fundamental physical and geometrical constraints. These models aim to reproduce the key features of biological evolution, including replication, inheritance of multiple traits, and adaptation.

One possibility is that Darwinian started at the molecular level with autocatalysts - molecules capable of amplifying their own production - playing the role of elementary replicators. To investigate this possibility, we tackled in recent years three related problems: (i) understanding the design principles of elementary catalysts, which are able to accelerate chemical reactions without complex mechanisms [2]; (ii) identifying what distinguishes enzymes - the molecular catalysts essential for nearly all reactions in modern cells - from these simpler chemical catalysts [3]; (iii) elucidating the design principles of simple autocatalysts and the conditions under which they may compete for common resources in a manner reminiscent of natural selection [4].

Despite autocatalysts demonstrating reproduction and selection, it remains unclear how they could generate the diverse, heritable variations necessary for extensive evolution. Inspired by models in theoretical ecology [5], we are currently developing a novel class of models in which systems of coupled chemical reactions can exhibit key features of Darwinian evolution - diversity, selection, inheritance, and adaptation - even in the absence of autocatalysis [6]. Our goal is to further develop this model to understand how additional features of Darwinian evolution might emerge. For example, we want to explore how the distinction between species and individuals might arise, a feature currently missing from our model.

The internship will involve both analytical and numerical calculations using concepts and methods from statistical physics. While no prior knowledge of Darwinian evolution is required, a genuine curiosity in the subject is expected. The work will be theoretical but our models are designed with potential implementations in soft matter, chemistry, or synthetic biology in mind, and there may be opportunities to collaborate with experimentalists.

The internship will take place in a diverse group of theoreticians and experimentalists whose backgrounds span physics and biology. The group shares a broad interest in molecular evolution and a common approach based on statistical physics. The work will be done in collaboration with Guy Bunin of the Technion in Israel, a specialist in theoretical ecology from a statistical physics perspective.

References:

[1] N. Goldenfeld, C. Woese (2011). *Life is physics: evolution as a collective phenomenon far from equilibrium.* Annu. Rev. Condens. Matter Phys., 2 : 375-399.

[2] O. Rivoire (2020). *Geometry and flexibility of optimal catalysts in a minimal elastic model*. J. Phys. Chem. B 124 : 807-813 ; M. Muñoz-Basagoiti, O. Rivoire, Z. Zeravcic (2023). *Computational design of a minimal catalyst using colloidal particles with programmable interactions*. Soft Matter, 19 : 3933-3939.

[3] O. Rivoire (2023). *How flexibility can enhance catalysis*. Phys. Rev. Lett. 131 : 088401 ; O. Rivoire (2024). *A role for conformational changes in enzyme catalysis*. Biophys. J. 123 : 1-16

[4] Y. Sakref, O. Rivoire (2024). *Design principles, growth laws, and competition of minimal autocatalysts.* Comm. Chem. (in press) ; Y. Sakref, O. Rivoire (2024). *On the exclusion of exponential autocatalysts by sub-exponential autocatalysts.* J. Theo. Bio. 579 : 111714.

[5] G. Bunin (2021). *Directionality and community-level selection*. Oikos, 130 : 489-500.

[6] G. Bunin, O. Rivoire (2024). *Evolutionary features in a minimal physical system: directionality, diversity, selection, inheritance, and adaptation.* (in preparation)