Master 2: *International Centre for Fundamental Physics*

INTERNSHIP PROPOSAL

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Thesis possibility after internship: YES
Funding: Ecole Doctorale EDPIF

Thermodynamics of autocatalytic chemical networks

Autocatalysis, the ability of chemical systems to make more of themselves, is a hallmark of living systems, as it underlies metabolism, reproduction, and evolution. Autocatalysis is also a primitive form of replication, which is likely to have played an essential in the origin of life. Recently, we have developed a theoretical framework for autocatalysis based on stoichiometry. This theory lead to the identification of essential motifs of autocatalytic networks, namely, autocatalytic cores, which come in five categories [1]. We also showed that compartmentalisation significantly adds diversity and evolvability in autocatalysis [2,3].

In this internship, we would like to understand the thermodynamics and the dynamics of autocatalytic chemical networks. One difficulty in this task is that often only coarse-grained (i.e. global and non-elementary) information is available about chemical networks. Nevertheless, recent progresses in non-equilibrium statistical physics and Stochastic Thermodynamics offer solutions to model chemical networks and address this issue. With these methods, we plan to analyse the role of thermodynamic constrains for the emergence and maintenance of autocatalysis, and investigate how these features are connected to the motifs present in autocatalysis. Such a thermodynamic analysis should also be useful to understand force-fluxes relations in the network, which characterise the system on a global scale, and are related to remarkable properties like robustness, adaptability and evolvability. This project should also benefit from interactions with a group of researchers from the lab or from nearby institutes and interested in related topics : Z. Zeravic and Y. Rondelez (Gulliver), P. Nghe (LBC lab) and O. Rivoire (Collège de France).

References :

[1] Universal motifs and the diversity of autocatalytic systems, A. Blokhuis, D. L. and P. Nghe, PNAS (2020) :
https://www.pnas.org/content/early/2020/09/25/2013527117
[2] Selection dynamics in transient compartmentalization, A. Blokhuis, D. L., P. Nghe and L. Peliti, Phys. Rev. Lett., 120, 158101 (2018).
[3] Reaction dynamics in open reactors and serial transfers between closed reactors, A. Blokhuis, D. L. and P. Gaspard, J. Chem. Phys., 148, 144902 (2018).