Emergent computational abilities of chemical reaction networks

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Possibilité de thèse: Oui
Financement: Non

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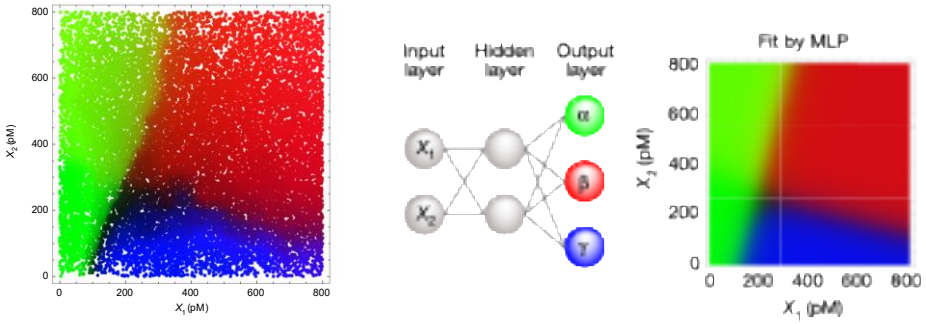

Left: Fluorescence plot showing a classification task performed by an enzymatic chemical network (x1 and x2 are concentrations of DNA strands). Right: classification task performed with a perceptron using two layers (both figures from Ref [3]).

Summary

We propose to study strategies to control chemical reaction networks, in order to use them to perform computations, with certain similarities to the computations by biological or artificial neural networks. In these systems, certain properties can be emergent when they arise from the interactions of a large number of components. In the group, we have studied previously two such properties, homochirality [1] and autocatalysis [2] and we have found that their emergence is indeed favored in large chemical networks. We are now interested in new emergent properties, related to the ability to perform some form of computation. Computation should be understood here as the ability of the chemical network to dynamically reach a certain final composition given an initial composition. The computation should be robust, which means that a small perturbations in the kinetics of chemical reactions should not affect the final composition.

An experimental demonstration of a classification task using molecular chemical networks based on DNA has recently been realized by two members of the lab Y. Rondelez and G. Gines [3]. Inspired by this work, we propose to formalize theoretically and study numerically control strategies of molecular chemical networks based on DNA (or possibly RNA). The control parameters are here template molecules, which can be autocatalytically amplified and are typically in competition with each other. By viewing these templates as weights to be optimized, modern machine learning methods may be used for this problem.

What is the optimal architecture to do this, specially when the number of neurons is large ? Is there one choice of architecture which is optimal from the point of view of energy consumption [4], given that any computation necessarily requires some amount of dissipation. How can such networks learn? To address all these questions, we rely on recent methods of non-equilibrium Statistical Physics, Stochastic Thermodynamics and Machine learning. This theoretical internship will benefit from interactions with experimentalists in the lab and abroad.

[1] Emergence of homochirality in large molecular systems, G. Laurent, D. Lacoste, and P. Gaspard, Proc. Natl. Acad. Sci. U.S.A., 118, (2021)

[2] Universal motifs and the diversity of autocatalytic systems, A. Blokhuis, D. D. Lacoste, and P. Nghe, PNAS, 117, 25230 (2020).

[3] Nonlinear decision-making with enzymatic neural networks, S. Okumura et al., Nature, 610, 496 (2022).

[4] Structural constraints limit the regime of optimal flux in autocatalytic reaction networks, A. Despons et al., Commun. Phys. (2024)

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