Emergent computational abilities of chemical reaction networks

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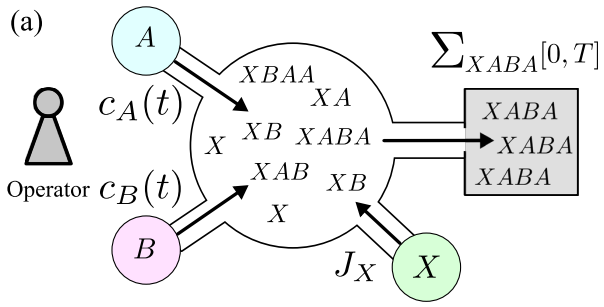
We propose to study strategies to control chemical reaction networks, in order to use them to perform computations, with certain similarities to the computations by biological or artificial neural networks. In these systems, certain properties can be emergent when they arise from the interactions of 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 as illustrated in the figure. We are interested in robust computations in the sense 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 to 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 but 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.

The goal of this internship/thesis is to understand how to best control chemical reaction networks. We ask what are the fundamental limits in the computation power of such networks. These limits may depend on the topology of the chemical network or on thermodynamic constraints [4], because any computation necessarily requires some amount of dissipation. To address 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.



By introducing template molecules at appropriate times a control in the output of a chemical network can be achieved, with the final composition playing the role of the result of a computation with respect to the input composition. Figure from I. Kobayashi et al., PRL (2022).

References:

[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)