Contingent dynamics in unbounded chemical networks: towards the emergence of prebiotic Darwinian processes

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From the standpoint of evolutionary biology, understanding the origin of life amounts to understanding how natural selection may arise in a non-biological world governed by purely physico-chemical processes (1). Meeting this goal requires an explicit articulation of evolutionary theory with physics and chemistry. Yet the problem remains challenging, since the basic ingredients of evolutionary thinking – populations of self-replicating objects displaying heritable variation – are still to be fully formulated in a prebiotic framework (2, 3). One promising approach relies on mathematical modelling: simulating open systems that obey the fundamental laws of thermodynamics and tracking dynamical behaviours that could be interpreted as emerging Darwinian processes.

In this context, our team has developed a first model, focusing primarily on the behaviour of autocatalytic cycles within predefined and bounded chemical networks connecting fixed sets of chemical objects through fixed sets of reactions (4). Ongoing projects in our group now investigate how autocatalytic cycles may interact in complex ways, akin to ecological relationships, potentially generating a broad diversity of steady states and paving the way to incipient Darwinian dynamics. While this framework helps clarifying important first principles, it may also overlook a critical property of the real world, where life has actually emerged: the immense diversity of possible chemical objects – especially macromolecules or supramolecular assemblies – produced by contingent trajectories representing only a minute fraction of the virtually infinite space of possibilities.

The goal of the proposed internship is to overcome these limitations by designing and exploring a new modelling approach, in which only chemical rules are initially specified, generating unbounded chemical networks expanding gradually and stochastically in an infinite chemical space. We anticipate that explicitly considering a finite number of discrete particles will be an effective way to implement this framework: in this context, chance effects will naturally come into play, and only a subset of all possible trajectories will be explored. In these simulations, concentration vectors will change dynamically through a combination of deterministic and stochastic processes, producing dynamics that may be only partly repeatable. Given the crucial role of chance in biological evolution, we expect this new modelling scheme will bring us closer to understanding how natural selection should be conceived beyond the standard biological context. Practically, the software will be developed as part of our existing EmergeNS platform (5), a C++ program integrating an efficient command-line interface and a user-friendly graphical environment with advanced visualisation features.

The research will be carried out within a dynamic group, including recently recruited PhD students and postdoctoral researchers, currently working on ecological-like relationships between autocatalytic sets and on the multistability of chemical networks – two directions that will help interpret the simulation results.

We are looking for a highly motivated student interested in interdisciplinary approaches, with skills in computational or mathematical modelling and a strong interest in evolutionary biology. The internship is part of the ANR-funded EmergeNS project (starting early 2026), which involves groups at LIP (Laboratoire de l'Informatique du Parallélisme, with Denis Kuperberg, ENS Lyon), LBBE (Laboratoire de Biométrie et Biologie Évolutive, with Etienne Rajon, University of Lyon), and PIMIT (Processus Infectieux en Milieu Insulaire Tropical, Reunion Island, with Sylvain Charlat, CNRS). The strong links between partners ensure a stimulating and truly interdisciplinary environment, bridging mathematics, physics, ecology and evolutionary biology. The internship will take place at the LBBE. Opportunities for continuation as a PhD project at PIMIT or LBBE will be discussed.

References

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