The ecology of autocatalytic cycles, in the context of the origin of life

Autocatalytic cycles, that is, ensembles of chemical compounds that can collectively self-amplify, are seen as putative key players in the origin of life, or more generally, in the physico-chemical emergence of Darwinian dynamics. Without directly displaying heritable variance in fitness (the necessary condition for evolution by natural selection) these objects nevertheless engage in rudimentary ecological dynamics that may pave the way toward evolution. Some cycles can't run simultaneously, because they rely on incompatible chemical conditions, while others may interact through competitive or synergistic relationships. To investigate these dynamics, it is necessary to articulate physical, chemical and biological concepts, with the appropriate mathematical tools. The present internship proposal relies on such a framework that we have recently developed, introducing thermodynamic constraints in the detection and depiction of autocatalysis.

One current objective is to better characterize, using numerical solvers, the topological and thermodynamic properties of reaction networks that make two autocatalytic cycles incompatible. We have already shown that two cycles may be incompatible simply because they require opposite reactions, or more subtly because they rely on incompatible stoichiometric constraints, imposed by thermodynamics. A more exhaustive search of such incompatibilities remains to be achieved, with the goal of developing a predictive typology. A second short term objective is to use simulations to investigate the joint dynamics of compatible cycles in an ecological framework, that is, to better understand if, and why, autocatalytic cycles may interact competitively, or in contrast in a synergistic fashion. Depending on the skills and inclinations of the applicants, each of these directions, or both, may be included as objectives of this internship.

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