Network science to study the emergence of complexity in the origin of life

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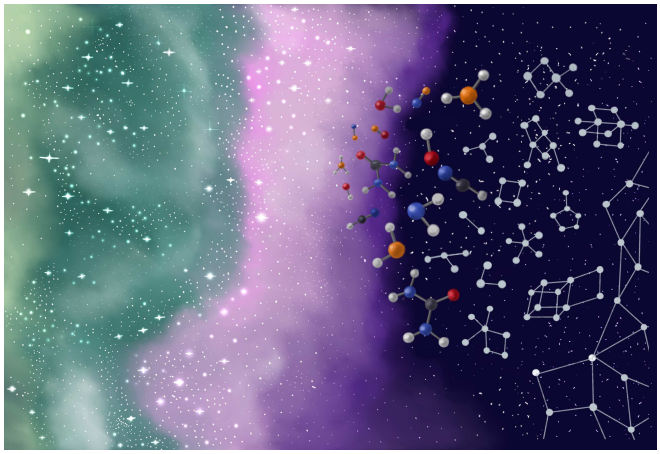
The road to life is punctuated by transitions toward complexity, from astrochemistry to biomolecules and eventually, to living organisms. Disentangling the origin of such transitions is a challenge where the application of complexity and network theory has not been fully exploited. Encouraged by this idea, we present a theoretical and computational framework, NetWorld, to model the evolution of simple networked structures toward complexity [1, 2].

In our computational environment, simple networks simulate the most basic building bricks of life and interact to form complex structures. The framework unveils the emergence of a drastic transition from simple structures toward complexity when the parameter representing the environment reaches a critical value. Notably, although our system does not attempt to model the rules of real chemistry nor is dependent on external input data, the results describe the emergence of complexity in the evolution of chemical diversity in the interstellar medium, where the original blocks of life could have been produced before being introduced in the early Earth by asteroids and meteorites during the Late Heavy Bombardment that took place between 4.1 and 3.8 billion years ago.

In particular, our results describe the real abundance distributions of chemical compounds detected in four interstellar clouds, and where a transition towards complexity takes place when the amount of interstellar dust (or extinction, playing the role of the environment parameter of our model) reaches a critical value and protects the cloud from the external interstellar UV radiation [3]. Furthermore, our work reveals an as yet unknown relationship between the abundances of molecules in dark clouds and the potential number of chemical reactions that yield them as products, supporting the ability of the framework presented here to shed light on real scenarios.



In summary, our work builds a bridge from complexity to astrobiology and reinforces the notion that some of the properties that condition the extremely complex journey from the chemistry in space to prebiotic chemistry and finally, to life could show relatively simple and universal patterns.

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[1] M. García-Snchez, I. Jiménez-Serra, F. Puente-Sánchez and J. Aguirre, *The emergence of interstellar molecular complexity explained by interacting networks*, PNAS **119** (30), e2119734119 (2022).

[2] `https://github.com/MiguelGarciaSanchez/NetWorld`

[3] M. Agúndez and V. Wakelam, *Chemistry of dark clouds: Databases, networks, and models*, Chem. Rev. **113**, 12, 8710 (2013).