An artificial chemistry towards the identification of the transition to life

Ivan Alfredo Mendoza, Patricia Muethe, Jonatan Gómez and Marcela Ewert-Sarmiento

National University of Colombia
iamendozap@unal.edu.co

A simplified model of a natural system in the form of an Artificial Chemistry is presented in order to explain the origin of life. It is intended to serve as a tool for modelling certain scenarios where conditions that could lead to the formation of the compounds, thought to have a major role in the emergence of life, are met. The "molecules" (first element of an Artificial Chemistry) in this model take the form of two-dimensional atoms modelled after those most commonly found in living creatures (with a justification for their inclusion). These atoms have specific shapes (and places for bonds) for metals, nonmetals and metalloids. Their last energy level valences, electronegativities, radii (based on the Helium radius along with all other distances in the system) and weights are also included in the model. The rules were designed with two main purposes, to move the atoms around the reactor and to make and destroy bonds. In this way, molecules are formed, moved around and eventually they give form to new molecular species too. Atoms are initially placed at random over a two dimensional space and also given an initial random velocity and acceleration. Their movement is based then in one of two alternatives, since no forces can be modelled to move the atoms in this level: the first approach is to give them velocities that change depending on their relationship (bonding potential) with others in the neighbourhood. The second alternative is to randomly accelerate them but keeping a total constant value for this acceleration, proportional to the atomic weight. For bonding purposes a novel approach is introduced. It is based on a combined strategy that involves the electronegativity difference between two atomic species (when free valences are available) and the "gross affinity", a magnitude given for two specific atomic species that was obtained from counting real bonds from a database of bioorganic molecules. This gross affinity favours the formation of compounds that can be familiar in the context of the origin of life, so the future work for this model is based on the fine-tuning of initial conditions (quantities, placing and environment division) and the modification of the affinity to make the model to move towards specific desired results. Also, the emergence of a prevalence of more complex structures and behaviours could be achieved by tracking down the processes that eventually led to them, boosting these processes with new rules can be a form of mimicking natural selection. The preliminary results are optimistic in terms of the production of basic molecules and substrates and compounds as the ones found in experiments like the ones conducted by Miller and Urey.