

Stochastic Cellular Automata models simulating Early Earth prebiotic self- organization reactions

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Geochemical reactions in multi-phase systems of Early Earth were essential prerequisites for the formation, polymerization, compartmentalization, and self-proliferation of the first biomolecules[1]. We don't know for sure which reactions lead to the emergence of life. Chemical gardens, a famous example of purely inorganic biomorphic precipitates, are considered among possible geochemical routes for early life emergence[2]. Although these systems are well-studied, the mechanisms of their formation are not understood in detail. Cellular Automata (CA) algorithms provide a great opportunity to model the formation of chemical gardens by introducing rules for reactions based on local neighborhoods[3]. The power and beauty of CA models is their ability to capture the global dynamics of complex systems describing only local interactions. CA models simulate the behavior of different systems and phenomena: pattern formation in reaction-diffusion systems, phase transitions, crystal growth and dissolution, intercellular interactions in multicellular organisms, avalanches, and forest fires. Most known CA models are deterministic, as Steven Wolfram originally introduced them in the 1980s. Although they can generate complex, intricate patterns and describe many phenomena, the patterns are always the same at given initial conditions[4]. In contrast, most natural systems have intrinsic stochastic components that might sometimes be necessary to consider. The kinetic Monte Carlo is an example of a stochastic CA algorithm, where micro-statistics of events are simulated via introducing kinetics in probabilistic forms[5]. I show here how stochastic CA can be utilized for modelling various systems characterized by pattern formation and self-organization: silica gardens, chemical waves in reaction-diffusion systems, cell-cell communication in biological tissues, as well as systems mimicking multi-phase materials characteristic for the prebiotic environment of Early Earth. I discuss the common dynamical features characteristic of inorganic and organic systems, which may provide some clues for prebiotic reaction pathways.

References: [1]Garcia-Ruiz, van Zuilen, and Bach (2020), *Phys. Life Rev.* 34-35, 62-82; [2]Garcia-Ruiz et al. (2017), *Science Advances* 3 (3), e1602285; [3]Batista et al. (2024), *PNAS* 120 (28), e2305172120; Wolfram (2002) *A New Kind of Science*, [5]Kurganskaya and Luttge (2021), *ACS Earth Space Chem.* 5 (7), 1657–1673.