COMPUTATIONAL INSIGHTS INTO THE EMERGENCE OF REPLICATION, HEREDITY, AND SPECIATION IN ABIOTIC SYSTEMS

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Introduction: Contemporary biology exhibits many phenomena whose emergence from non-living systems have been studied but not yet fully explained, such as replication, heredity, and speciation [1-5]. The emergence of these phenomena leads to specific questions fundamental to understanding the origins of life before the hereditary architecture of modern genes first evolved. In particular, how is diversity generated or maintained in prebiotic systems? What characterizes a line of descent? How does information propagate forward through time?

Laboratory research has been conducted to investigate these questions, perhaps most directly through a synthetic chemical system composed of self-replicating fibers that compete for molecular building blocks [5]. This system is capable of non-templated replication, providing a novel model for heredity in abiotic systems. Aside from replication, this system is found to exhibit other features normally associated with biology, such as speciation, and mutation. Due to the nature of this laboratory work, instrument limitations restrict the amount of information that can be extracted from the system, stymieing our understanding of the mechanisms driving the emergence of these `life-like' features.

We conduct computational simulations based on the model of this synthetic chemical system, featuring the reactions hypothesized to be occurring *in-vitro*, in order to fully record the features of the system which cannot be probed using laboratory analytics. Here we present the features uniquely investigated by our computational simulations, including preliminary results as they apply to the open questions posed above.

Model construction: The model used as the basis for our computational simulations is composed of two building blocks (A and B monomers), which can undergo oxidation reactions to form trimers [5]. Trimers may exchange monomers to change composition, or combine to form a hexamer and free monomer. Hexamers may degrade back to trimers, or nucleate to form a fiber. Fibers may elongate or fragment. See Fig. 1 for description of model reactions. The fragmentation process is what we refer to as fiber replication.

Simulation construction: We use the Gillespie Algorithm, a variant of the Kinetic Monte-Carlo algorithm [6], in order to simulate the stochastic chemical evolution of the model system. The propensity for each reaction is proportional to the concentration of the reactants, and the reaction's rate constant. A reaction is simulated every time step, chosen by a probability distribution weighted by reaction propensities.

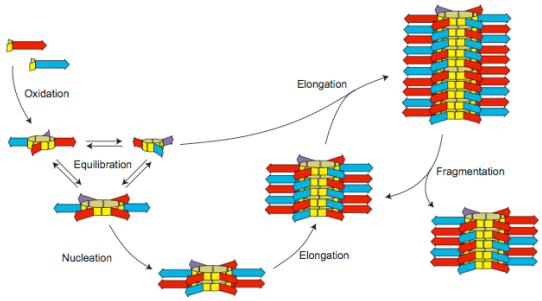

Figure 1. Reactions present in the modeled abiotic chemical system. Fibers are composed of hexamers, and replicate through fragmentation, a non-templated process. Figure adopted from [5].

System properties probed through model simulations: Simulations can probe how exactly the differential interaction of A-A, A-B, and B-B bonds affect longitudinal fiber composition, and what role this plays in the changing composition of the fiber as it elongates. Knowledge of fiber composition can be used to study how fiber fragmentation (replication) engages in non-templated information transfer, leading to a better understanding of non-genetic mechanisms of heredity and speciation in a purely synthetic, abiotic system. Complete knowledge of the systems molecules can further be used to study how fiber composition and growth is affected its chemical environment. Future plans will study change to molecular diversity over time with the goal of uncovering long term, stable patterns in the evolution of the system.

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