Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Physical polymerization mechanisms in the chemistry-to-biology transition.

By

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Studying complex systems and emergent phenomena is very popular today. The reason is that we desperately need more knowledge about many complex systems such as cells, organisms, society, emergent phenomena on the internet. Applying physical and quantitative methods to such systems resulted in many discoveries. Yet a lot of knowledge is missing. In particular, we don't fully understand living systems including their emergence. What are the minimal requirements for life? How to make a chemical system capable of inheritance and an open ended evolution? If a system is capable of Darwinian evolution, is it necessary a living system? Modern life relies in its functioning (including inheritance and capability to evolve) on long polymeric molecules: proteins and nucleic acids. Because of their indispensable role in cells it is very important to understand the origins of these biological polymers as well as their role in the emergence of inheritance, evolution and metabolism. Are long biological polymers enough to jump-start life? We propose physical mechanisms of emergence of long bio-polymers in the prebiotic world. We use HP lattice model to model polymerization, interaction and folding of short chains of hydrophobic (H) and polar (P) monomers. We show that such chains fold into relatively compact structures exposing hydrophobic patches. These hydrophobic patches act as primitive versions of modern protein's catalytic site and assist polymerization of other HP-sequences. These HP-sequences form autocatalytic, self-sustaining dynamic systems capable of multimodality: ability to settle at multiple distinct quasi-stable states characterized by different groups of dominating polymers. We study properties of these systems to see their role in the chemistry-to-biology transition. We also propose a stochastic simulation algorithm for modeling agent-based complex systems, in particular polymeric systems with several types of monomers. This algorithm is efficient for the sparse systems: systems where the number of the species which could possible be generated is much higher the the number of species actually generated, thus it allows for simulation of the systems with unlimited number of molecular systems.

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