

A First-Principles Model of Early Evolution

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In a study publishing in *PLoS Computational Biology*, Shakhnovich et al present a new model of early biological evolution – the first that directly relates the fitness of a population of evolving model organisms to the properties of their proteins.

Key to understanding biological evolution is an important, but elusive, connection, known as the genotype-phenotype relationship, which translates the survival of entire organisms into microscopic selection for particular advantageous genes, or protein sequences. The study of Shakhnovich et al establishes such connections by postulating that the death rate of an organism is determined by the stability of the least stable of their proteins.

The simulation of the model proceeds via random mutations, gene duplication, organism births via replication, and organism deaths.

The authors find that survival of the population is possible only after a “Big Bang” when a very small number of advantageous protein structures is suddenly discovered and exponential growth of the population ensues. The subsequent evolution of the Protein Universe occurs as an expansion of this small set of proteins through a duplication and divergence process that accompanies discovery of new proteins.

The model resolves one of the key mysteries of molecular evolution – the origin of highly uneven distribution of fold family and gene family sizes in the Protein Universe. It quantitatively reproduces these distributions pointing out their origin in biased post “Big Bang”

evolutionary dynamics of discovery of new proteins. The number of genes in the evolving organisms depends on the mutation rate, demonstrating the intricate relationship between macroscopic properties of organisms – their genome sizes – and microscopic properties – stabilities – of their proteins.

The results of the study suggest a plausible comprehensive scenario of emergence and growth of the Protein Universe in early biological evolution.

Citation: Zeldovich KB, Chen P, Shakhnovich BE, Shakhnovich EI (2007) A first-principles model of early evolution: Emergence of gene families, species, and preferred protein folds. PLoS Comput Biol 3(7): e139. doi:10.1371/journal.pcbi.0030139
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