



Mini Review

Computing the origin and evolution of the ribosome from its structure – Uncovering processes of macromolecular accretion benefiting synthetic biology

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ABSTRACT

Accretion occurs pervasively in nature at widely different timeframes. The process also manifests in the evolution of macromolecules. Here we review recent computational and structural biology studies of evolutionary accretion that make use of the ideographic (historical, retrodictive) and nomothetic (universal, predictive) scientific frameworks. Computational studies uncover explicit timelines of accretion of structural parts in molecular repertoires and molecules. Phylogenetic trees of protein structural domains and proteomes and their molecular functions were built from a genomic census of millions of encoded proteins and associated terminal Gene Ontology terms. Trees reveal a 'metabolic-first' origin of proteins, the late development of translation, and a patchwork distribution of proteins in biological networks mediated by molecular recruitment. Similarly, the natural history of ancient RNA molecules inferred from trees of molecular substructures built from a census of molecular features shows patchwork-like accretion patterns. Ideographic analyses of ribosomal history uncover the early appearance of structures supporting mRNA decoding and tRNA translocation, the coevolution of ribosomal proteins and RNA, and a first evolutionary transition that brings ribosomal subunits together into a processive protein biosynthetic complex. Nomothetic structural biology studies of tertiary interactions and ancient insertions in rRNA complement these findings, once concentric layering assumptions are removed. Patterns of coaxial helical stacking reveal a frustrated dynamics of outward and inward ribosomal growth possibly mediated by structural grafting. The early rise of the ribosomal 'turnstile' suggests an evolutionary transition in natural biological computation. Results make explicit the need to understand processes of molecular growth and information transfer of macromolecules.

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1. Introduction

“As we trace the changes in structure or function back through time, we must bear in mind that all of the structures and functions of the cell may be simpler. We are then dealing with primitive components ancestral to those seen today.” Eck and Dayhoff [1]

Galaxies evolve by accretion, gravitational interactions, harassment, and dry and wet mergers of stars, gas and dust clouds [2]. Stars form by gravitational collapse within giant molecular clouds and accrete circumstellar disks of orbiting matter that spiral inward towards the growing central bodies [3]. Planets arise from the proto-planetary disks of gas and solids by a process of accretion and N-body interactions [4]. Unsurprisingly and at the other end of the spectrum, macromolecules in the biological world arise and evolve by similar processes of accretion,

adding component parts to growing molecules, which also interact and merge with other molecular bodies to form molecular complexes and repertoires and higher order molecular and cellular structure.

The dynamics of macromolecular accretion involves a number of agents of genetic change, including point mutations, insertions, deletions, rearrangements, fusions, and fissions, and a multiplicity of interactions that prompt nucleating foci for growing molecules. While some of these processes materialize relatively quickly in lineages of organisms others take millions to billions of years to unfold. Their rates and distributions are not well understood. The protein world for example is incredibly vast when studied at polymer sequence level but its diversity can be currently summarized with only ~1200 fold designs that distil the fundamental topologies of their atomic 3-dimensional (3D) structures [5,6]. Amino acid sequences showcase a limited alphabet that changes constantly by mutation. Sequences become saturated with recent mutations. They are poor repositories of historically deep phylogenetic information. In contrast, the structure of proteins and nucleic acids

Table 1
Glossary of selected terminology.

| Term | Definition |
|---|--|
| Character | In phylogenetics, a character is an observable feature of a biological entity (primary homology) that is used to establish its history. Characters have alternative manifestations (character states) and are most powerful when they unfold as 'shared and derived' features (synapomorphies) in evolutionary tree or network hypotheses. |
| Character transformation | A series of character states that transform into each other in evolution. |
| Character polarization | Assignment of polarity to a character transformation. Polarity implies specifying direction of character change and which states are evolutionarily ancestral and which are derived. Character polarization enables the rooting of phylogenetic trees or networks and the identification of synapomorphies. |
| Dynamical system | A natural object delimited by a set of interacting component subsystems, which is characterized and individuated from other systems by its cohesion [11]. Cohesion refers to the dynamical stabilities of the components of the system, its parts, when these are constrained by the system as a whole. Consequently, systems are by definition decomposable into subsystems that are either spatially bounded (e.g. nucleotides in nucleic acids) or spatially unlinked (e.g. processes or other dynamical entities). Cohesion is the property of modules, a special group of parts. |
| Hennigian argumentation | An explicit procedure of retrodiction that uses character transformations (evolutionary models) and phylogenetic information in individual characters (data) to build tree or network hypotheses of evolution |
| Hennigian (reciprocal or mutual) illumination | A successive approximation route for developing scientific theories of evolution, in which additional evidence in the form of more informative phylogenetic characters is added to a corpus of ideographic evidence to support the validity of phylogenetic hypotheses. |
| Finite state machine | A mathematical model of computation conceived as an abstract machine (black box) that can be in one of a finite number of states, one state at a time. A state can transition into another state induced by a stimulus or input. A typical example is a coin-operated turnstile with two-states (locked and unlocked) and two inputs (insert coin and push turnstile mechanical arm). See Fig. 4. |
| Frustrated dynamics | Patterns of change and behaviors of systems governed by competing and often opposing forces. Examples of frustration include spin glasses, which are important for condensed matter physics. In biology, RNA folding for example follows a frustrated dynamics, in which structural conformations that are formed are both stabilized by hydrogen bonding interactions between bases and destabilized by unpaired regions of the molecules. |
| Laplacian demon | Pierre Simon Laplace in his <i>Essai philosophique sur les probabilités</i> (1814) articulated the rationale of causal or scientific determinism: “We may regard the present state of the universe as the effect of its past and the cause of its future. An intellect which at a certain moment would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes.” His demon represents a utopian super-intelligence capable of perfect foreknowledge. |
| Lundberg rooting | A method of rooting that first determines an optimal tree or network and then adds a hypothetical ancestor (defined by all-ancestral state characters) at the position in the tree or network that is most optimal. |
| Matrix transposition | Mathematical operation in which a matrix is converted into a new matrix whose rows are the columns of the original. |
| Node | A point in a phylogenetic tree or network where three or more branches meet. |
| Phylogeny | A hypothesis of genealogical relationships among a group of entities (taxa) in the form of a tree or network with specific connotations of ancestry and an implied time axis. |
| Ribosomal translocation | Movement of the codon-anticodon duplices on SSU from A and P sites to the P and E sites, respectively [112]. |
| Weston's generality criterion | A general criterion of character polarization capable of distinguishing ancestral and derived character states. The criterion, inspired by Nelson's ontogenetic rule, states: “Given a distribution of two homologous characters in which one, x, is possessed by all of the species [taxa] that possess its homolog character y, and by at least one other species that does not, then y may be postulated to be apomorphic [derived] relative to x.” It is based on homology and additive phylogenetic change, and is most powerful when features of characters accumulate 'iteratively' in evolution (e.g. gene paralogs via duplication). |

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