Process-based Modelling of RNAs and Proteins towards the Simulation of Long-distance Electrodynamic Interactions in Biomolecules

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Our work is focussed on the computational study of the molecular interactions in biological systems. We hypothesise the use of process algebras to highlight the relation between the complexity of the functions carried out by a biological entity and the type of interactions tying the elementary units that compose its structure. This approach is intended to define predictive models able to generate new knowledge, on the system itself, complementary to the one obtained via empirical methods.

We investigated the way in which the interactions between nucleotides determine the three-dimensional conformation of RNAs and hence their functions. With the aid of formal models based on process algebras, we compared the folding process of proteins with the one performed by RNAs. We formally proved the existence of an abstraction level in which these two kinds of processes show a congruence in their behaviour. Such result allows us to identify and model the distinguishing features of the studied biological processes only on the basis of the known properties of the interactions that bind the nucleotides (in RNAs) and the amino acids (in proteins). This was possible thanks to the expressiveness of a specific process algebra, the Milner's CCS (Calculus of Communicating Systems)[1].

We are also working on an application of the proposed modelling approach to the studies carried out at the CPT (Centre de Physique Théorique, Aix-Marseille University), on the long-distance electrodynamic interactions of biomolecules[2]. The main idea is to develop a simulator able to solve the problem of the possible interpenetrations of the represented molecules. It would be also intended to yield information on the temporal evolution of the molecular interactions.

Applications of our approach in modelling the processes involved in the gene expression would allow the identification of mutations in human gene pathologies; on the other hand, simulations of protein interactions would be the basis of in-silico studies of the formation of protein aggregates, like amyloid plaques in neurodegenerative diseases.

References:

1) Milner, R. Communication and Concurrency; *Upper Saddle River*, **1989**, *NJ, USA: Prentice-Hall, Inc.*

2) Gori, M. et al. Investigation of Brownian diffusion and long-distance electrodynamic interactions of biomolecules. *Noise and Fluctuations (ICNF)*, **2015**, *International Conference on. IEEE*, pp. 1 – 4.