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On two ways to predict the protein folding process over a chaotic model

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In our first theoretical studies about folded self-avoiding walks, we have raised several questions regarding the protein structure prediction problem and the current ways to solve it. In one category of PSP software, the protein is supposed to be synthesized first as a straight line of amino acids, and then this line of amino acids is folded out until reaching a conformation that optimizes a given scoring function. The second category considered that the protein is already in the aqueous solvent, and it does not wait for the end of the synthesis to take its 3D conformation. So they consider SAWs whose number of steps increases until the number of amino acids of the targeted protein end. At each step, the current walk is stretched (one amino acid is added to the protein) in such a way that the pivot k placed in the position that optimizes the scoring function. We have proven that the two sets of possible conformations are different. So these two kinds of PSP software cannot predict the same kind of conformations. We have proven too that the folding process G in the 2D model is chaotic according to Devaney. A consequence of this theorem is that this process is highly sensitive to its initial condition. If the 2D model can accurately describe the natural process, then this theorem implies that even a minute difference on an intermediate conformation of the protein, in forces that act in the folding process, or in the position of an atom, can lead to enormous differences in its final conformation. In particular, it seems very difficult to predict, in this 2D model, the structure of a given protein by using the knowledge of the structure of similar proteins. Let us remark that the whole 3D folding process with real torsion angles is obviously more complex. And finally, that chaos refers to our incapacity to make good prediction, it does not mean that the biological process is a random one.

Figure1: *A conformation that cannot be reached by a folding process on the straight line.*

Biography

Christophe Guyeux has a record of about 120 scholarly publications. Since 2010, he published 43 articles in peer-reviewed international journals (as a co-author, including the top-ranked ones in the areas of Computer Science and interdisciplinary applications, such as AIP Chaos, PLOS ONE, and Clinical Infectious Diseases). He is a co-author of 2 book chapters and 2 scientific monograms. He is also author of 4 software patents, 53 articles that appeared in proceeding of peer-reviewed international conferences. His topics for research encompass Bioinformatics, discrete dynamical systems, and information security. He is currently working as Full Professor at Femto-ST Institute, Université de Bourgogne Franche-Comté, France.

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