Structural proteomics: Do computers help?

Carlos Polanco*

Department of Mathematics, Faculty of Sciences, Universidad Nacional Autónoma de México, México City, éxico

Accepted on February 03, 2018

Introduction

Characterizing the structure of proteins is a fundamental issue for understanding the biological systems in all living creatures. Presently, the study of the structural properties of proteins is based on mathematical computational software that automatically read protein databases [1] noted as amino acids or nucleotides. Multiple codes simultaneously evaluate the primary or tertiary structure of proteins with different mathematical algorithms that vary in degree of complexity [2]. These algorithms experimentally verify any regularity, and 'virtually' build proteins from certain physico-chemical properties.

Things were very different 60 years ago, the work was done in University Labs, where after decades of endless work, a new protein or a physico-chemical property shared by a group of proteins were discovered. All that hard work, made possible to build the databases that today are the source of information used by these computer programs for protein structural analysis.

Are the romantic times when a scientist devoted his entire life to lonely search for a protein over? It seems they will continue because without this work it will not be possible to refine or improve the reliability of these databases. However, the introduction of computing to the study of protein regularities has welcomed a new group of scientists, as valuable as those working in laboratories. They are scientists specialized in the design and programming of computational mathematical algorithms [3] based on solid biochemical knowledge.

Why design mathematical algorithms that will later need a computational implementation to run on specific databases? The answer is not simple. The phrase "if something doesn't work, read the manual" cannot be easily applied here. Here, the user's manual will only be consulted if the computational code cannot run, otherwise, it will not be consulted. It can get even worse, if the manual is consulted it will probably state how to run the program, but will not describe the algorithm, or the programming language the algorithm has been written in. Then, how can we be sure that what the program produces is correct? The answer is: we cannot be sure. Today the pace of work and the pressure institutions put on scientists to obtain results does not allow the time to verify them.

The new stage on the analysis of structural regularities in proteins is still to be written, it will require committed scientists with solid knowledge in biochemistry, mathematics, and expertise in parallel computing, capable of programming in mathematical processors such as GPU, or FPGAs, in order to substantially reduce the processing time, without affecting the efficiency of the algorithm. These scientists will have to be able to participate in interdisciplinary groups. And they will probably become the new romantics that absorbed in their work, will see the nights pass by until the sunlight announces a new day.

Dr. Carlos Polanco is a mathematician with specialization in parallel computing, he has spent the last 15 years developing computational mathematical algorithms focused on Structural Proteomics. He is Associate Professor of the Department of mathematics of the Faculty of Science at the Universidad Nacional Autónoma de México.

References

1. UniProt Consortium. UniProt: A hub for protein information. Nucleic Acids Res. 2015; 43 204-12.
2. Romero P, Obradovic Z, Li X et al. Sequence complexity of disordered protein. Proteins. 2001; 1; 42 38-48.
3. Altschul SF, Gish W, Miller W et al. Basic local alignment search tool. J. Mol. Biol.1990; 215; 403-10.

***Correspondence to:**

Carlos Polanco
Department of Mathematics,
Faculty of Sciences,
Universidad Nacional Autónoma de México, México City,
México

Citation: *Polanco C. Structural proteomics: Do computers help? J Syst Biol Proteome Res. 2018;2(1):9*