INVITED TALK
COMPUTATIONAL BIOPHYSICS

METABOLIC SYSTEMS BIOLOGY: TOOLS FOR MODEL-BASED ANALYSIS AND DESIGN OF MICROBIAL SYSTEMS

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Industrial Biotechnology has been replacing chemical processes in numerous industrial sectors since it allows the use of renewable raw-materials and provides a more sustainable manufacturing base. The field of Metabolic Engineering (ME) has thus gained a major importance since it allows the design of improved microorganisms for industrial applications. However, in Metabolic Engineering problems, it is often difficult to predict the effects of genetic modifications on the microorganism, owing to the complexity of the underlying biological systems. Consequently, the task of identifying the modifications that will lead to an improved microbe is a quite complex one, requiring robust mathematical and computational tools.

In this presentation I will introduce the main framework of the in silico design of improved microbial strains and will focus in some of our group’s efforts in these fields, namely in the development of improved mathematical models of metabolic and regulatory processes and the development of reliable and effective computational methods for the design of rational metabolic engineering strategies. Furthermore, I will introduce the open-source software tool developed in house, called OptFlux (www.OptFlux.org), that allows researchers both from industry and academia to simulate, in a user-friendly way, the behavior of microorganisms under a variety of conditions and also indicates which genetic modifications may lead to enhanced strains for a particular application or which are the putative essential genes that can be used as drug targets, in the case of pathogens.

Bridges with established and emergent fields such as structural biology and enzyme engineering will also be explored.

Keywords: Systems Biology. Metabolic Models