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A flux balance approach to integrate cell metabolism into multicellular agent-based simulations

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Abstract

The study of multicellular systems such as tumors, tissues, or organoids is critical to improve our understanding of the complex dynamics exhibited by these systems. For instance, the emergence of resistant cancer cells is process that manifest at many different scales from the molecular, to the population level. Multicellular systems such as tumors are complex adaptive systems an thus are no reducible to classical analytical techniques. Nevertheless, multi-scale simulations can used study these systems by integrating models of processes taking place at these different scales. In this way, multi-scale model simulations provide a genotype-to-phenotype mapping framework, that allow the exploration of genetic variations and their interaction with changing environmental conditions. In the Computational Biology Group we are extending a multiscale modelling

framework combining agent-based and models of signaling pathways (PhysiCell/PhysiBoSS), to link pathways' activity and cells' phenotypes to physical interactions among cells and with their environment. In this seminar, I will introduce the current status of our multi-scale framework, as well as the ongoing development of a novel extension to integrate metabolic models within the agent-based framework. This novel feature will allow to study the intersection between cell metabolism and their microenvironment, at the population.

Short bio

Dr. Miguel Ponce de León is a postdoctoral researcher at the Computational Biology Group at the Life Science Department of the BSC. His background is in the field of systems biology , scientific computation, and most of his research has been on reconstruction and simulation of biological network models. From 2011 to 2017, he was the academic coordinator of the Master degree in Bioinformatics and Computational Biology (ISCIII-ENS), where he has also been teaching Linux and Python programming for bioinformatics.

His current research line at the BSC is the development of systems biology approaches to personalized medicine, with a particular focus on cancer. For this purpose, he uses different modeling approaches to integrate heterogeneous sources of omic data with two main objectives: 1) to develop tools to assist in the decision-making process of choosing the most adequate therapy for specific patients, given their unique genetics/background; and 2) to improve our knowledge of basic cancer biology.