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Objectives

Abstract: Computational simulations of cellular processes (e.g. metabolism, gene expression, signal transduction) are critical tools to formulate mechanistic explanations that facilitate the interpretation of experimental results. However, complex biological processes such as tumour evolution span across different time-space scales. For instance, a population-level description is needed to account for genetic heterogeneity and phenotypic variability due to environmental noise, whereas intracellular models, such as cell signalling networks need to address the effect of mutated genes. In this context, multi-scale models are ideal tools to address systems biology questions as they can consider several time-space scales by combining different approaches into a hybrid simulation.

PhysiCell is an open-source, agent-based extensible multi-scale modelling framework that allows simulating complex multicellular systems such as healthy tissues and tumours. At the lowest scale, PhysiCell uses BioFVM solver to simulate the chemical microenvironment using partial differential equations which model the diffusion, uptake and secretion of substrates and signalling molecules. At the cell scale, PhysiCell uses mechanical equations to model individual cell movement, cell-cell interactions, as well as interactions between cells and the microenvironment's physical components, e.g. as extracellular matrix. Additionally, different cells types and heterogeneous populations can be defined by using different submodels for cell growth, death as well as user-defined custom behaviours.

Furthermore, PhysiCell can be extended to provide cell agents with more complex intracellular networks, such as signalling and metabolism. For instance, PhysiBoSS is an addon-based extension that provides cell agents with individual Boolean models of regulatory networks which are simulated using the MaBoSS algorithm. The Boolean model inputs can be connected to different cell variables and their outputs can be used to trigger changes in the cell behaviour. Altogether, PhysiBoSS bridges intracellular dynamics to the population level. Because of its flexibility, the PhysiCell Framework can be applied to a broad range of biological problems related to cancer, immunology, infectious diseases, and microbial ecology, among others. In this webinar, we will introduce the basic concepts of the PhysiCell/PhysiBoSS modelling framework and its HPC-based implementation using different biological examples focusing on applications to treatment optimisation in models of tumour growth.



Short bio: Miguel Ponce de León is a recognised postdoctoral researcher at the

Computational Biology Group at the Life Science Department of the Barcelona Supercomputing Center

(BSC). His area of expertise is in the field of systems biology and scientific computation where most of his research has been on reconstruction and simulation of biological networks. His line of research at BSC is the development of systems biology approaches to personalised medicine, with a particular focus on cancer. He uses different modelling approaches to integrate heterogeneous sources of information with two main objectives: 1) developing tools to assist in the decision-making process of choosing the most adequate therapy for specific patients given their unique genetic/background; and 2) improving the knowledge of basic cancer biology.

We hope you will find this topic interesting and will join us for this second session. We would like to remind you that this webinar is the second of a set of PerMedCoE webinars that are open to everyone interested in our tools and activities.

The webinars will include a 30-40 minutes presentation and a Q&A section of around 15 minutes. You will find all webinars here: <https://permedcoe.eu/category/training/> and you are able to register for free. All PerMedCoE webinars will be made available on the [dedicated playlist on the project's YouTube channel](#).

Speakers

Miguel Ponce de León, Barcelona Supercomputing Center (BSC)

Learning Outcomes

Describe the PhysiCell modelling framework using biological examples

Explain how PhysiBoss bridges intracellular dynamics to the population level

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