Cell Level Simulations and Digital Twins

S-04.6-2

A. Valencia[I]

[I]Plaza Eusebi Güell 1-3, Spain, Spain

In this presentation, I will address the area of simulations of cell behaviour that include molecular networks, pathways and cellular interactions, covering the space between atomistic simulations, based on Molecular Dynamics and system level simulations of organs, based on fluid dynamics equations.

PerMedCoE (HPC/Exascale Centre of Excellence in Personalised Medicine, [1] has developed a framework (PhysiBoSS [2]) that combines agent based simulations of cell interactions in the context of a given environment (PhysiCell, [3]) with Boolean simulations of biological pathways (MaBoSS, probabilistic Boolean framework [4]) implemented in each cell.

We have tested the capacity of these models to use as input genomic information, from bulk to single cell data, to provide mechanistic molecular models and testable hypothesis on different biomedical scenarios. Use cases include simulations of COVID infection on layers of epithelial cells or the simulations of temporal evolution of tumours and their micro-environments in response to genomic alterations or drug treatments.

In the final part, I will discuss the possible avenues for the integration of cell level simulations in the context of larger systems including digital twins of human organs and the potential application in areas of personalised medicine and preclinical trials [5].