SCALABLE AGENT-BASED MODELLING OF CELL BIOMECHANICS AND THERAPY USING THE BIODYNAMO PLATFORM

Vasileios Vavourakis (1,2), Roman Bauer (3)

1. University of Cyprus, Cyprus; 2. University College London, UK; 3. University of Surrey, UK

Introduction

In silico models in computational cell biomechanics are usually confronted with the fact that they need to capture processes across multiple spatial/temporal scales. These processes play out intracellularly, such as for instance gene regulatory dynamics, as well as extracellularly, such as their interactions with the extracellular matrix and parenchymal components. Moreover, intercellular processes often play a crucial role too, particularly during growth and developmental phases. Agent-based modelling (ABM) alone, or via hybrid multiscale procedures, is an attractive approach to explore complex biological processes. Here, we demonstrate ABM in biomedical applications using open-source simulation platform BioDynaMo [1]. We present a selection of examples to demonstrate the simulation of biological cell growth and development, therapy, and cell pathophysiology in chronic diseases.

Methods

ABM is a complex-system modelling method that assumes autonomous, interactive 'agents' that are denoted as a particles (cells) or segments (neurites, vessels), positioned in 2D/3D-space following an off-lattice approach, and 'agent behavior' is determined by rules as a Markov process. Our ABM platform, BioDynaMo, can encompass the interactions with other cells and response to external stimuli, their ability to secrete or/and uptake cytokines, enzymes, etc. The open-source project BioDynaMo, implements ABM and it has been designed to leverage modern software engineering techniques and enables high-performance computing using OpenMP, MPI and CUDA [1].

Results

The following figures illustrate the applicability of the ABM platform, BioDynaMo, through four simulation examples in cancer and wound healing/inflammation.

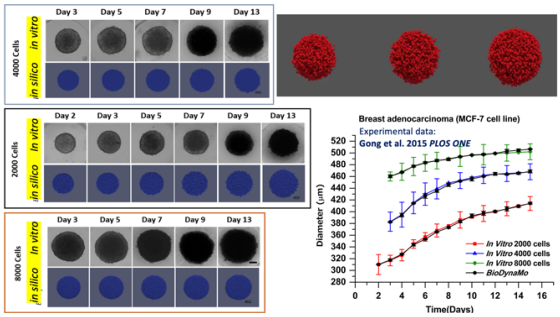

Figure 1: ABM simulation, using BioDynaMo, of a monoculture cancer spheroid (breast adenocarcinoma MCF-7) growth in a free-suspension medium [1].

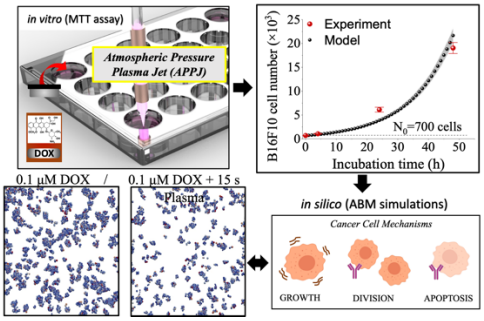

Figure 2: ABM to simulate cancer cell death due to cytostatics, or combined with atmospheric plasma [2,3].

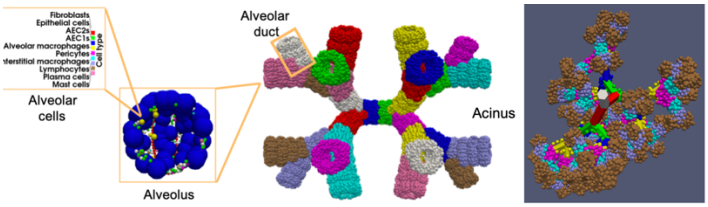

Figure 3: Hybrid ABM of alveoli, alveolar ducts, and acini to simulate radiation-induced lung fibrosis [4].

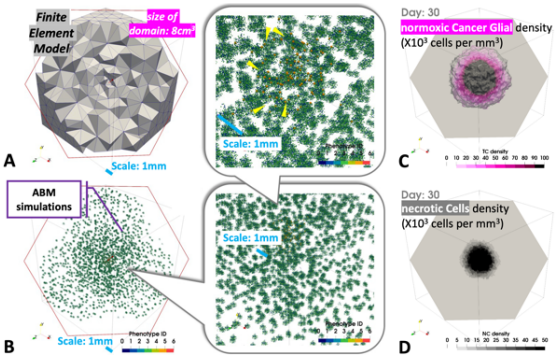

Figure 4: Coupled multiscale FEM / ABM simulation of an in situ glioblastoma tumor growth [5].

Discussion

We have demonstrated the BioDynaMo platform to simulate the development cancer by mimicking *in vitro* systems, to simulate the effect of cytostatics and other treatment modalities, and to simulate the patho-physiology of diseases such as pulmonary fibrosis. BioDynaMo is available at www.biodynamo.org.

References

1. Breitwieser et al. Bioinformatics, 38:453-460, 2022.
2. Gazeli et al. Applied Physics Letters, 120:054101, 2022.
3. Demetriades et al. Pharmaceutics, 14:749, 2022.
4. Cogno et al. Symmetry, 14:90, 2022.
5. de Montigny et al. Methods, 185:94-104, 2021.

Acknowledgements

We are very grateful for the contributions of all BioDynaMo consortium members, the technical team, and the alumni.