Capturing Spatial Constraints and Stochasticity in Innate Immunity: Translating an ODE Model to a Cellular Potts Framework Using CompuCell3D

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We present the translation of a simple deterministic ODE model of the innate immune response to a 2D rules-and-physics-based Cellular Potts model in the open source software package CompuCell3D. A Cellular Potts model (CPM) is a computational model that can be used to simulate the behavior of cells and other biological entities. CPMs are based on the idea that cells can be represented as discrete objects that interact with each other according to a set of rules. These rules can be used to simulate a variety of biological processes, such as cell growth, division, and death. The goal of this translation is to first conceptualize immune cell interactions in a spatial framework that includes spatial constraints and components such as cellular adhesion, secretion, and exposure to extrinsic factors such as chemical fields. To begin, we focus on macrophage phenotype switching in two settings, homeostasis and under exposure to varying levels of LPS, as a means of validating model behavior against expectations. In this simple context, we describe the energy formalism of the CPM, illustrate how simulations are written using Python steppables and XML, show how model outputs are tracked and visualized, and how model parameters are estimated.