



Biocellion: Accelerating multicellular biological simulation

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Biological phenotypes of interest commonly result from complex, multicellular systems. From hundreds of cells that determine micro-environments to the billions of cells that make up complex organs. At the same time cellular and molecular biologists have unveiled intricate details on the intracellular processes that drive cell behavior and decision-making. Bridging this gap, between microscopic and macroscopic scales, is a critical challenge in systems biology. One potentially powerful tool is multiscale agent based modeling. With this strategy, discrete agents, such as cells, are computationally modeled on a high-resolution grid, which represents the extracellular space. However, the computational complexity can often force modelers to use low-resolution approximations of the biological system. To this end, we have developed Biocellion, a multicellular modeling framework that takes advantage of high-performance parallel computing. Biocellion relieves the modeler of common, yet complex computational problems allowing for computational efficiency and scalability over multiple cores and machines. In this presentation, we will present the details of this new modeling platform in the context of two examples that demonstrate the computational power and flexibility of Biocellion. First, we will describe the implementation of an epidermal skin model described in the literature. We will demonstrate how Biocellion can be used to produce significant speed up of the simulation. This improved performance gives us the ability to increase the size and complexity of the model, which is important in simulating clinically relevant systems. Secondly, we will describe the use of Biocellion in modeling and design of microfluidic chips for the study of budding yeast. This study demonstrates the ability for Biocellion to quantitatively describe systems with complex geometries at the micrometer length scale. Finally, we will discuss future plans for Biocellion to help foster adoption in the community and provide high performance computing solutions to new, multicellular modeling challenges.