## Somogyi\_2019 ML-MSM Meeting - Abstract Submission Form

**Title: Multi-Cellular Model Specification and Simulation**

**PI(s) Grant: N/A**

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**Title of Grant: Competitive Renewal of Development, Improvement and Extension of the Tissue Simulation Environment - CompuCell3D, Dissemination of libRoadRunner and CompuCell3D**

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**Abstract Text:**

Biological cells are the prototypical example of active matter. Cells sense and respond to mechanical, chemical and electrical environmental stimuli with a range of behaviors, including dynamic changes in morphology and mechanical properties, chemical uptake and secretion, cell differentiation, proliferation, death, and migration. Modeling and simulation of such dynamic phenomena poses a number of computational challenges. A modeling language describing cellular dynamics must naturally represent complex intra and extra-cellular spatial structures and coupled mechanical, chemical and electrical processes. Traditional computer programming languages, which describe sequences of ordered operations on data, however are not well suited to describing the simultaneous parallelism of biological phenomena.

In order to be relevant and relatable to biomedical professionals, modeling and simulation of biological cells, tissues and materials requires a natural description of biological objects, behaviors, and interactions, to allow flexible, automated model specification and automated interconnection between computational solvers.

Mapping high-level biological descriptions, which are often incomplete and inconsistent to mechanistic implementation is significant research challenge. Machine learning optimization approaches manipulate model structures and parameters, as such, they need a machine understandable model structure format.

To address these challenges, we are developing a modeling language that is both human and computer understandable, which separates biological behaviors from the underlying chemical and mechanical aspects, and we are implementing a hybrid vertex / particle -based simulation engine. This language enables both domain experts and machine learning systems to define models using natural, biologically motivated constructs and to simulate time evolution of coupled cellular, mechanical and chemical processes acting on a time varying number of cells and their environment.

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