VCell: Spatial Modeling, Reactions and Rules

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VIRTUAL CELL (VCELL) is a general modeling and simulation framework for cell biology. Modeling with VCell allows simultaneous consideration of biochemistry, membrane transport, electrophysiology and diffusion. It can be used for non-spatial compartmental deterministic (generating and solving systems of ODEs) and stochastic (using stochastic Gibson and hybrid methods) simulations; when spatial effects cannot be ignored, VCell can simulate reaction/diffusion/advection within 1D, 2D and 3D geometries deterministically (generating and solving systems of PDEs) and stochastically (using the SmolDyn simulator). VCell is freely available at http://vcell.org. Any simulation can be run locally on a user's computer, or sent to VCell servers where multiple jobs can be submitted and run, with both model and simulation results stored in VCell database and available to the user and his/her collaborators.

In this tutorial I will demonstrate the full range of VCell capabilities, demonstrating how a reaction network can be specified and simulated using compartmental deterministic and stochastic simulations, how an arbitrary geometry can be specified in VCell using different methods (specifying it analytically, based on experimental image, or using constructive solid geometry), and how a spatial model can be simulated using deterministic or stochastic algorithms.

I will demonstrate special features of the VCell, such as using a Pathway Commons collection of pathway databases (http://pathwaycommons.org) to create and annotate models of biological systems, and a new graphical interface to specify rule-based models and run them using the network generation capabilities of BioNetGen (http://bionetgen.org) and the network-free simulation capabilities of NFSim (http://nfsim.org). The new interface allows a modeler to design a rule-based model without scripting in the BioNetGen Language. A distinct feature of the VCell rule-based capabilities is the option to mix and match reaction network and rules in a single-compartment model.