Smoldyn

a spatial stochastic simulator for chemical reaction networks

What Smoldyn is

Smoldyn is a computer program for cell-scale biochemical simulations. It simulates each molecule of interest individually to capture natural stochasticity and to yield nanometer-scale spatial resolution. It treats other molecules implicitly, enabling it to simulate hundreds of thousands of molecules over several minutes of real time. Simulated molecules diffuse, react, are confined by surfaces, and bind to membranes much as they would in a real biological system.

Smoldyn is easy to use and relatively easy to install. It is more accurate and faster than other particle-based simulators. Smoldyn's unique features include: a "virtual experimenter" who can manipulate or measure the simulated system, support for spatial compartments, molecules with excluded volume, and simulations in 1, 2, or 3 dimensions.

News

Smoldyn 2.29 released April 10, 2013

- Minor bug fixes from version 2.28
- Rule-based modeling is more functional
- Pre-compiled code and improved build system

Smoldyn in Virtual Cell

- VCell 5 runs spatial-stochastic simulations using Smoldyn

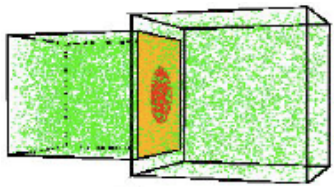
Upcoming talks

- June 19 in Seattle at SASB 2013

Updated simulator citation figure

- See this figure.

Research Highlight



Membrane and actin reorganization in electropulse-induced cell fusion

Günther Gerisch, Mary Ecke, Ralph Neujahr, Jana Prassler, Andreas Stengl, Max Hoffmann, Ulrich S. Schwarz and Eberhard Neumann, *J. Cell Science* 126, 2013

Electric pulses induce *Dictyostelium discoideum* cells to fuse. The authors combined electron microscopy, fluorescence microscopy, and simulation to study the fusion pores and actin localization that arise in the membrane during cell fusion. They found that the plasma membranes of the contiguous cells become tangles of highly bent and interdigitated membranes. By imaging GFP diffusion from one cell to its neighbor, and then modeling this diffusion with Smoldyn simulations as shown in the figure, they found that membranes persist in a fusogenic state for up to 24 seconds before pores of about 3 nm are formed.

Smoldyn is written and maintained by Steve Andrews. Development has been supported by the National Institutes of Health, the U.S. Department of Energy, the National Science Foundation, and the MITRE Corporation.