Abstract
Smoldyn is a simulator for modeling molecular diffusion, chemical reactions, and molecule-membrane interactions with nanometer scale resolution. It represents molecules as individual spherical particles in 1, 2, or 3-dimensional continuous space. Smoldyn is very accurate, easy to install, and easy to use. It is widely used for simulating cell systems and biophysical problems.

New features include: (1) rule-based modeling for simulating protein modification and complexion, which Smoldyn simulates using either the formal BioNetGen language, or a new informal wildcard method, (2) improved excluded volume algorithms for simulating macromolecular crowding, (3) better support for particle tracking, and (4) hybrid simulation capabilities for faster runtimes.

Smoldyn is open source and available for free at http://www.smoldyn.org.

Core Smoldyn

Diffusion. Simulated with Gaussian-distributed random displacements on each coordinate. Can also simulate drift, anisotropic diffusion, and diffusion on surfaces.

Surface interactions. Molecules can reflect, adsorb, desorb, or transmit through surfaces with user-definable rate coefficients.

Chemical reactions. Two molecules react when they end up within a binding radius of each other at the end of a time step. When a molecule dissociates to two products, those products are separated by an unbinding radius to control the probability of geminate recombination.

Biophysics studies

Multi-site phosphorylation

Macromolecular crowding

Cell division diffusion barriers

Network expansion with BioNetGen.

L(c12r) + R(r2m) <-> L(c12r) + R(r2m) bklon,brloff
K(DP)+M(soln) <-> K(DP)+M(soln) rsmon,rsloff
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Network expansion with wildcards. Models can also define reaction "rules" using a new wildcard method. Wildcards specify species groups much like operating system wildcards specify groups of files. This is generally simpler than BioNetGen, but inferior for large networks.


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Typical uses

Cell systems

Neural dendritic spines

E. coli chemotaxis

E. coli Min system

Apoptosis

Nuclear tethering

Yeast cell signaling

Rule-based modeling

Problem. Proteins that can be post-translationally modified (e.g. phosphorylated) and/or form multimeric complexes can produce a large number of variations. This leads to a lot of chemical species and reactions.

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References