Stochastic modeling and simulation of cell signaling using StochSim

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StochSim is a stochastic simulator of chemical reactions written in C++, and is particularly suited for studying cell signaling pathways involving multiprotein complexes. Accurate simulation of such pathways is difficult with conventional deterministic methods, because of (a) the very large number of possible reactions due to combinatorial effects, (b) the sensitivity to the stochastic behavior of low-concentration molecules, and (c) the effects of spatial organization of molecules within the cell. To deal with (a) and (b), StochSim version 1.0 (Windows) uses a discrete object-oriented representation of individual molecules, capable of storing their internal states, and a unique stochastic algorithm developed by Carl Firth. Further development of StochSim to address (c) is underway, and version 1.2 (Linux/Windows), featuring a two-dimensional spatial representation for simulating protein aggregates on the membrane has been released.

Future plans for StochSim development include the implementation of a more realistic spatial representation for simulating three-dimensional diffusion, improving the representation of molecular complexes to support nested complexes, and porting of the GUI for Linux/UNIX operating systems.