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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 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 2.31 released September 9, 2013

- Very minor bug fixes
- Several new runtime commands
- Surface panels can be moved mid-simulation

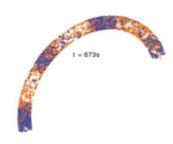
NSF proposal for Smoldyn development

- Submitted August, 2013.
- If funded, it will support development of methods for simulating filaments and multimeric complexes. It will also support ongoing collaborations.

Steve Andrews is on the job market

• See here.

Research Highlight



Oscillations of Min-proteins in micropatterned environments: a three-dimensional particle-based stochastic simulation approach

Max Hoffmann and Ulrich S. Schwarz, Soft Matter In press, 2014

One way in which E. coli bacteria find their mid-planes, so that cell division yields two equal size daughter cells, is with spatiotemporal oscillations of the Min proteins. These proteins oscillate from pole to pole, with minimal occupancy of the mid-plane. The simplicity and remarkable dynamics of this system has made it popular for spatial stochastic simulations. These authors investigated Min system operation in artificial micropatterned environments and in mutant filamentous cells, such as the one shown in the figure. This work highlights the robustness and variability of Min system oscillations, puts limits on the effect of putative division sites, and provides a computational framework for future studies.

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, albeit never by funding that was dedicated specifically for this purpose.



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