StochKit : A Stochastic Simulation Toolkit

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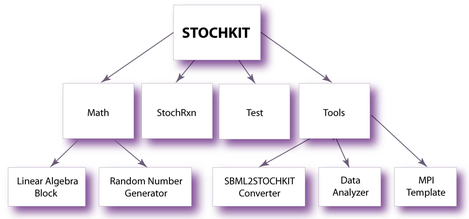
Abstract

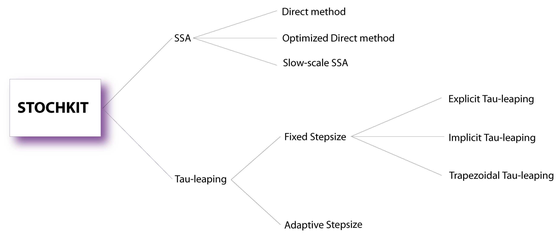
Traditional ordinary differential equation-based approaches to simulation of chemical reacting systems fail to capture the randomness inherent in such systems at scales common in intracellular biochemical processes. We present StochKit, an efficient, extensible stochastic simulation framework developed in the C++ language that aims to make stochastic simulation accessible to practicing biologists and chemists, while remaining open to extension via new stochastic and multiscale algorithms. The current version of StochKit has the basic simulation ability using the popular Gillespie SSA algorithm, optimized SSA algorithm, slow-scale SSA, explicit, implicit and trapezoidal tau-leaping methods. We provide a Java Converter to convert an SBML file specifying the chemical mechanism to the input files needed for our software. StochKit includes some basic tools to solve a question of great concern to developers of accelerated stochastic algorithms—how can we verify the accuracy of a stochastic solver, given the inherently random nature of stochastic simulation? The Kolmogorov distance and histogram distance for quantifying differences in statistical distribution shapes are provided in the Matlab language. For those who need to run the Monte Carlo simulations a large number of times to collect an ensemble, we provide a convenient MPI interface enabling the Monte Carlo simulation to run on a parallel cluster. Details can be found at http://www.engineering.ucsb.edu/∼cse.

Structure



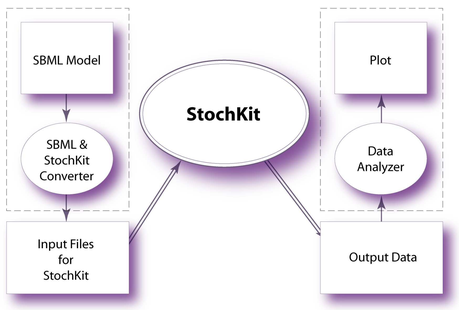
Math: This module provides a set of operations similar to the Matlab environment.
StochRxn: The core simulation functions that StochKit provides are included here.
Tools: StochKit provides three tools to make the stochastic simulation more convenient.
Test: StochKit provides this part to demonstrate and test the package.

Methods StochKit Supplies



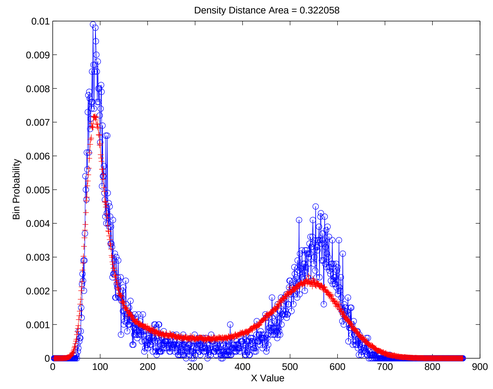
Direct Method: This is Gillespie's original SSA method, an exact stochastic simulation algorithm. [1]
Optimized Direct Method: This method includes an optimization to improve the efficiency of the direct method. [2]
Slow-scale SSA: This method is very efficient for systems containing both fast and slow reaction channels. [3]
Tau-leaping methods: This includes the original tau-leaping method [4], implicit tau-leaping method [5] and trapezoidal tau-leaping method. [6]

System Process



The ellipse represents software, the rectangle represents input, output or intermediate files.
StochKit: This is the main part of our StochKit package, an efficient, extensible stochastic simulation framework.
SBML2Stochkit Converter: This is a tool to convert the SBML model to the inputs of StochKit using Java.
Data Analyzer: This provides a capability for plotting distributions in the Matlab language.

Example



Histogram of Schlögl model simulated by SSA and explicit Tau-leaping methods. This plot is based on 10,000 samples of SSA runs and explicit tau-leaping runs with tau = 0.4.[7]

Others

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Weblink: Details can be found at http://www.engineering.ucsb.edu/∼cse .

References

[1] D.T. Gillespie. *J. Phys. Chem.*, 81:2340–2361, 1977.
[2] Y. Cao, H. Li and L. Petzold. 121(9):4059–4067, 2004.
[3] Y. Cao, D. Gillespie and L. Petzold. *J. Chem. Phys.*, 122:014116, 2005.
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