StochKit2: Efficient and extensible software for stochastic simulation of biochemical systems

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***Short Abstract* — Stochastic modeling and simulation is able to capture the inherent randomness present in cellular-scale biochemical systems. StochKit2 is an efficient and extensible stochastic simulation toolkit. It provides simulation methods and tools suitable for practicing biochemists, as well as a platform for stochastic simulation algorithm and software development.**

Details can be found at:
http://engineering.ucsb.edu/~cse/StochKit/

***Keywords* — stochastic simulation, software**

I. Background

TRADITIONAL deterministic models do not capture the inherent randomness of many biological processes featuring chemicals with low concentrations. On the other hand, the Chemical Master Equation (CME) is rigorously derived on a microphysical basis, and is often used to describe such models. Gillespie's Stochastic Simulation Algorithm (SSA) [1] generates exact trajectories of the CME. An estimate of the chemicals' distribution can be constructed by an ensemble of SSA runs.

Several algorithms have been proposed to speed up the SSA direct method: Optimized direct method [2], Logarithmic direct method [3], Constant time direct method [4], and others. Another approach is to sacrifice the exactness of the SSA to achieve greater efficiency gains. These methods include Tau-leaping [5, 6], Slow-scale SSA [7], and others.

II. StochKit2

We present StochKit2 as an efficient and extensible stochastic simulation software package. It features multiple solver options with implementations of several SSA algorithms with automatic selection of the fastest one. There is also a Tau-leaping method which adaptively selects step size and dynamically switches between SSA and Tau-leaping. All StochKit2 solvers feature automatic parallelism, utilizing multi-core technology for maximum efficiency.

Models for StochKit2 are represented in StochKitML, a simple XML-based format. It supports both mass-action reactions and reactions with custom propensity functions. Users can also use the SBML [8] converter included in the package to convert SBML models to StochKitML format.

StochKit2 has built-in support for SSA simulations with events. Events can be used to change the system state or parameter values to mimic biological processes or to recreate experimental conditions.

Simulation results can be stored as individual trajectories, statistics, and/or histograms. Matlab compatible functions are provided for visualization and analysis of trajectories and histograms.

III. Conclusion

StochKit2 features a simple and intuitive input format as well as a variety of efficient solvers. It also provides useful tools for importing existing SBML models and analyzing simulation results. StochKit2 is a valuable tool for practicing biochemists and provides a platform for algorithm and software developers.

StochKit2 is freely available for research use at:
http://engineering.ucsb.edu/~cse/StochKit/

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