Paweł Lachor
Institute of Informatics, Silesian University of Technology
e-mail: pawel.lachor@polsl.pl
Krzysztof Puszyński
Institute of Automatic Control, Silesian University of Technology
e-mail: krzysztof.puszynski@polsl.pl
Andrzej Polański
Institute of Informatics, Silesian University of Technology
e-mail: andrzej.polanski@polsl.pl

Accuracy indices for assessing performance of different versions of Gillespie Algorithm for stochastic molecular simulations

Dynamics in population models at the molecular level are commonly described using the deterministic approach based on systems of coupled first-order ordinary differential equations (ODEs). Deterministic approach although fast in calculation is not always accurate for systems containing low-rate reactions particularly for species occurring in small quantities. To account for random fluctuations in numbers of molecular species numerous variants of stochastic Gillespie Algorithm has been introduced. There are already several survey studies comparing and summarizing different approaches in stochastic modeling of molecular mechanisms. In these studies the problem of accuracy of modeling is addressed at the level of simplifying hypotheses and their verification [3], [4]. In our talk we critically discuss several possibilities of assessing accuracy of different strategies of stochastic molecular modeling. We also propose a new, direct and precise method of comparing different stochastic modeling strategies based on comparisons of probability distributions of observed time instants of molecular events. By using our methods we compare several variants of stochastic simulation methods, direct, approximate and hybrid (numerical integration of ODEs and stochastic simulation) [5], [6]. We grade accuracies of predictions of different algorithms in terms of differences betweeen conditional distributions of times of sequences of molecular events. In comparisons the basic version of the Gillespie algorithm is considered as an accurate one, predictions of other algorithms are analyzed based on its comparison to the basic version of the Gillespie Algorithm [1], [2]. Dedicated system written in C++ is used as a computational platform for calculation of models applying deferent approaches. Efficiency of system is also evaluated in comparison to common solutions.

Acknowledgment. This work was supported by the European Community from the European Social Fund.

Acknowledgment. This work was financially supported by The Fundation for Polish Science.

References

[1] D. T. Gillespie, *Exact stochastic simulation of coupled chemical reactions* The Journal of Physical Chemistry **81** 25.

[2] D. T. Gillespie, *Approximate accelerated stochastic simulation of chemically reacting systems* Journal of Chemical Physics **115** 4.

[3] J. Pahle, *Biochemical simulations: stochastic, approximate stochastic and hybrid approaches* Briefings in Bioinformatics **10** 53-64.

[4] Mario Pineda-Krch, *GillespieSSA: Implementing the Gillespie Stochastic Simulation Algorithm in R* Journal of Statistical Software **25** 12.

[5] E.L. Haseltine, J.B. Rawlings, *Approximate simulation of coupled fast and slow reactions for stochastic chemical kinetics* Journal of Chemical Physics **117** 15.

[6] K. Puszyński, R. Bertolusso, T. Lipniacki, *Crosstalk between p53 and NF-kB systems: pro- and anti-apoptotic functions of NF-kB* IET System Biology **3** 5.