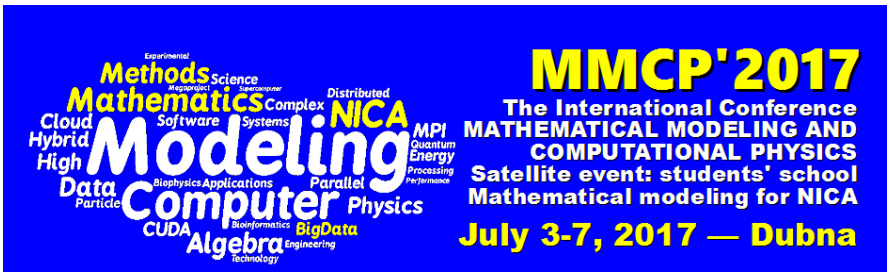

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Automation of stochastization algorithm with use of SymPy computer algebra library

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To describe models where the intensity of the interaction between components depends on the concentration of a component, one can use the scheme of interaction from chemical kinetics:
\[
\sum\limits^{n}{i=1}N^{s}{i}X_{i} \xleftrightarrow[\;\;k^{-}{s}\;\;]{\;\;k^{+}{s}\;\;} \sum\limits^{n}{i=1}M^{s}{i}X_{i},\; s = 1,\ldots,S.
\]
Here X_i represents the number i-th component, matrices $\mathbf{M} = [M_i^s]$ and $\mathbf{N} = [N_i^s]$ are called the system state matrices and specify the number of interacting components of the system at each stage of the reaction k_s^+ and k_s^- — are coefficients of interaction in direct and reverse reactions.
One can use such schemes to describe models of chemical reactions, biological and ecological systems. From these diagrams we can derive a system of ordinary differential equations describing the change of variables $X_i(t)$ over time.

Our research group has been generalized the stochastization method, which allows write out stochastic differential equation based on deterministic model . The original data reported in the interaction scheme, it is enough to get stochastic differential equations. For systems of large dimension, the stochastization method requires a large amount of routine work. However, it is possible to automate it. This paper describes this automation, by using Python language and SymPy library for symbolic camputations.

Created program allows from the array of the coefficients of the interactions to obtain at the output the system of ODE and vector drift and the diffusion matrix for the system of SDEs in human-readable form and in other formats suitable for direct numerical solution.

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Short biography note

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