Parallel stochastic reaction-diffusion simulation using Gillespie stochastic simulation algorithm

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ABSTRACT

Spatial stochastic simulation is a valuable method for studying processes of reaction and diffusion in biological systems. This technique requires significant computational efforts, but the availability of high-performance computing made it possible to develop coherent computational models of cells [1]. Several approaches were introduced in order to utilize parallel execution to speed up simulations. In [2] Gillespie multiparticle (GMP) method [3] was implemented, making use of GPGPU acceleration. This allowed significant computational speedup, reaching nearly the same accuracy as well-stirred simulations. Another approach was used in [4], where an attempt to develop parallel version of exact next-subvolume method using breathing time warp synchronization algorithm was made, resulting in moderate speedup.

Here a mixed approach is introduced. The simulated system is divided into cuboidal blocks, providing low level of unevenness in particle distribution between the blocks. Reaction-diffusion processes within a single block are simulated using exact next-subvolume method. Time difference between blocks is controlled by altering event generation in blocks exceeding threshold value, thus particles, diffusing between the blocks don't introduce significant noise. Simulation results compared with the results gained by exact methods show near the same accuracy. The developed method can be used to speed up stochastic simulations of reaction-diffusion processes in biological systems, facilitating modelling of cell structures.

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