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Stochastic simulation of reaction-diffusion processes in living cells on multiple scales

The number of molecules of each chemical species in biological cells is small and the molecules react with each other with a certain probability. A stochastic mesoscopic model of the diffusion and the chemical reactions is therefore more accurate than a deterministic, macroscopic model based on the reaction rate equations. In a computer simulation of a trajectory of the system, the diffusion is often the most computationally expensive part. The diffusion of different species are treated differently in [1] in order to reduce the computational cost. Depending on if the copy number is high, intermediate or low the diffusion events are simulated macroscopically, with the tau leap method or with the stochastic simulation algorithm (SSA) by Gillespie in an unstructured mesh covering the cell. The reactions are handled by SSA. Sometimes the mesoscopic model is not sufficiently accurate and a microscopic description is necessary. In such a model, single reacting and diffusing molecules are tracked [2]. The molecules move in the unstructured mesh by Brownian motion and are coupled to the mesoscopic model via the reactions [3]. Examples from molecular biology will be given.

REFERENCES

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