Universität Rostock

Traditio et Innovatio

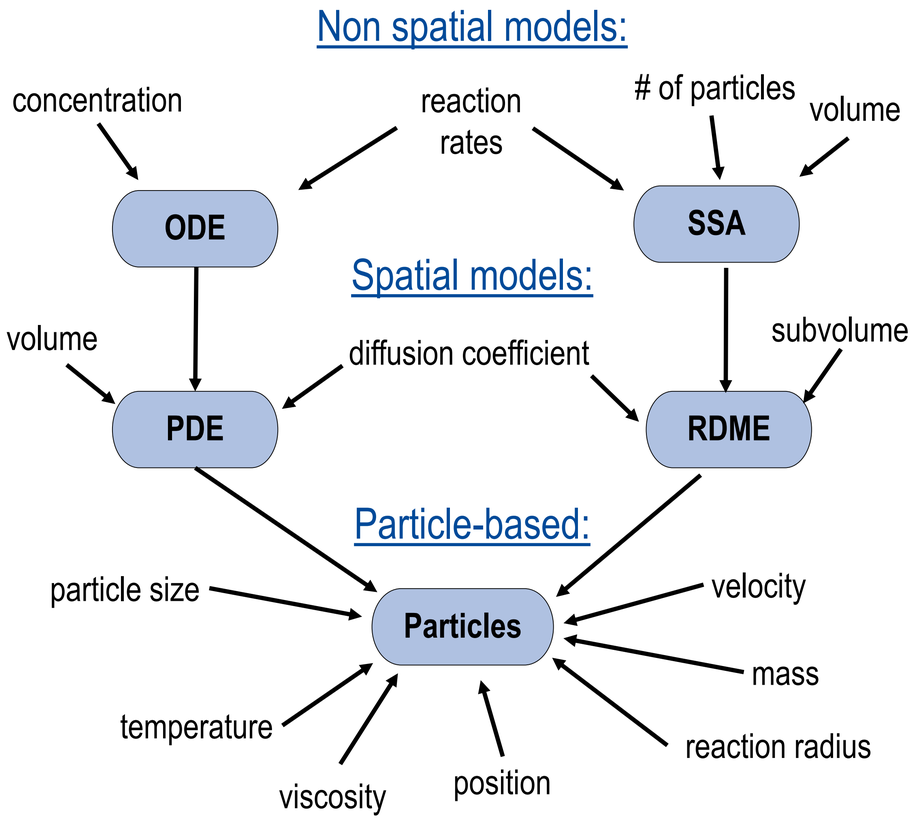
IDIOSYNCRACIES IN MULTI-SPATIAL MODELING

Philipp Henning, Till Köster and Adelinde M. Uhrmacher

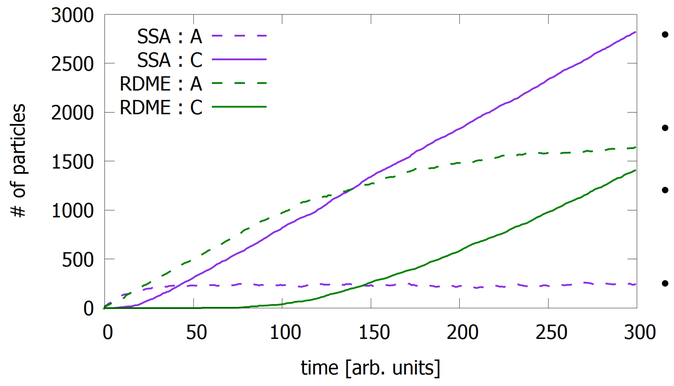
Motivation

Spatial models are an important tool to study cell biological processes. Different spatial simulation approaches offer different levels of spatial resolution to answer different questions of interest. These different levels require different information that has to be related to each other in moving from one level to the next. Based on a few small benchmarks we show possible implications of moving from one level to the next: from SSA to RDME and from ODE to two different particle-based approaches, one of which is a new development including compartments as well as forces [1].

Adding Spatial Aspects



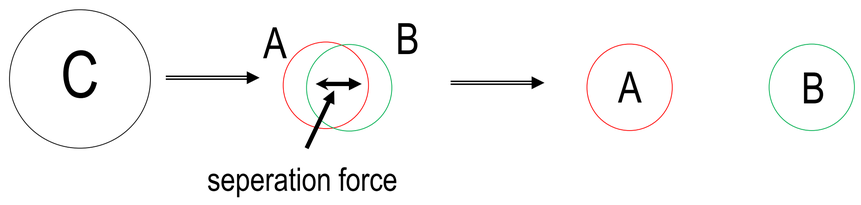
Comparison of SSA and RDME



- one source for A, one for B separated in space
- A + B ⟶ C
- higher amount of A and B in spatial simulation (RDME) vs. SSA
- Reason: delayed reaction due to spatial constraints

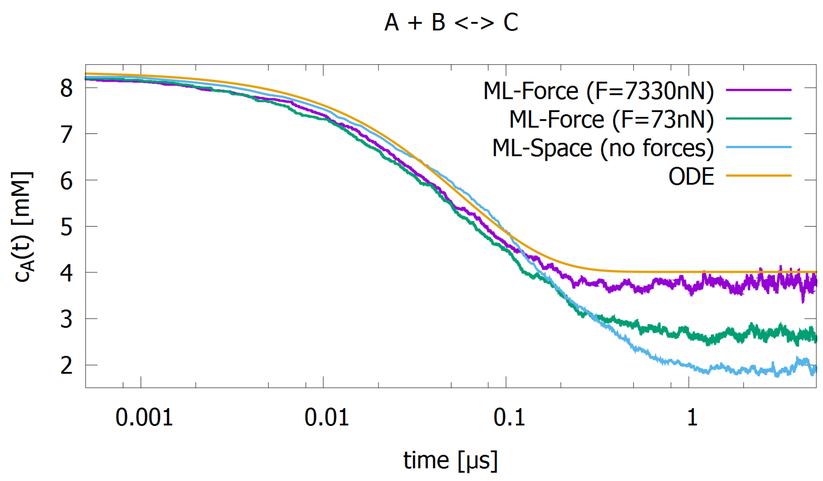
Reversible Reaction I

In a particle-based approach the handling of reversible reactions become an issue as shown in the example A + B ↔ C. After the dissociation of C the particles A and B are located nearby and hence very likely react back to C. In order to reproduce the correct equilibrium of such a reaction the particles are often displaced by a unbinding radius [2]. In our simulation tool ML-Force [1] we use separation forces to handle the dissociation in a more continuous manner.



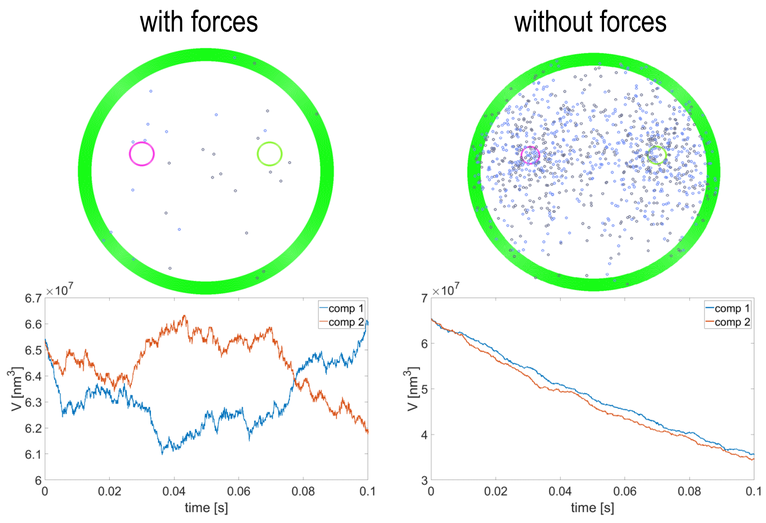
Reversible Reaction II

During the division the particles A and B are placed at the position of C. Then a separation force pushes them apart until they no longer overlap. The force can be adjusted to reach the right equilibrium.



Directed Movement

Biological processes often don‘t occur as a pure Brownian system since they are actively driven and directed, e.g. by a motor protein. These directed motion can be simulated in ML-Force by adding an external force as shown here with a vesicle transport between two compartments. By directed movements, the findings of [3] can be reproduced, as has also been shown in [4].



- Stable compartment size
- Few vesicles
- Directed motion

- Compartments shrink
- Many vesicles
- Undirected motion

References

[1] Köster, T. 2017. “Combined particle and compartmental dynamics of cell-biological models using hollow spheres on the GPU”. Master’s thesis, University of Rostock.
[2] Andrews, S. S., and D. Bray. 2004, September. “Stochastic simulation of chemical reactions with spatial resolution and single molecule detail”. Physical Biology 1 (3): 137–151.
[3] Heinrich, R. and Rapoport T. A. 2005, January. “Generation of nonidentical compartments in vesicular transport systems”. The Journal of cell biology, 168(2), 271-280.
[4] Michael Klann, Heinz Koeppl, and Matthias Reuss. 2012, January “Spatial Modeling of Vesicle Transport and the Cytoskeleton: The Challenge of Hitting the Right Road”. PLoS ONE, 7(1):e29645,

INSTITUTE OF COMPUTER SCIENCE | MODELING AND SIMULATION GROUP
University of Rostock, Albert-Einstein-Str. 22 | 18059 Rostock, Germany