Universität Rostock
Traditio et Innovatio

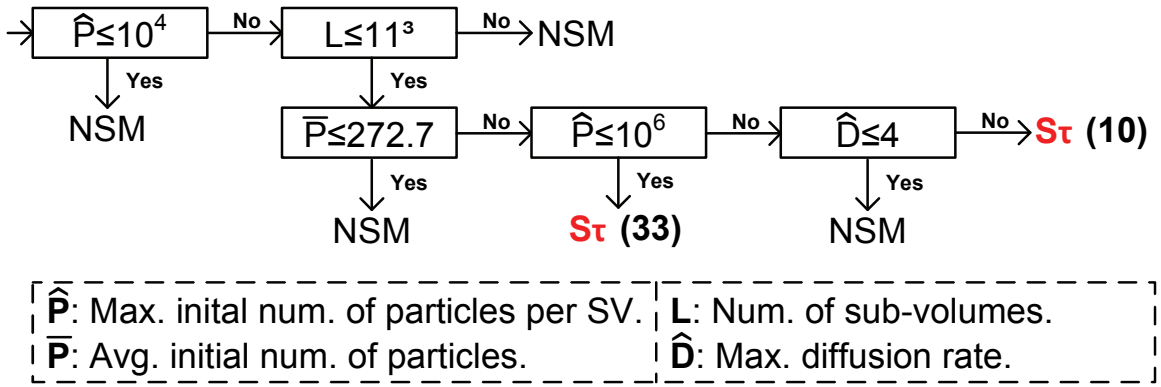
(Some) challenges for multi-level, spatial modeling and simulation

Adelinde Uhrmacher
University of Rostock
Institute of Computer Science

Challenge I - The OBVIOUS

Efficient execution of spatial models

- Partial differential equations are notoriously computational expensive.
- Can we expect better if taken the discrete spatial nature of cells into account and aiming for hybrid, approximate approaches?
- Or will we do even worse?

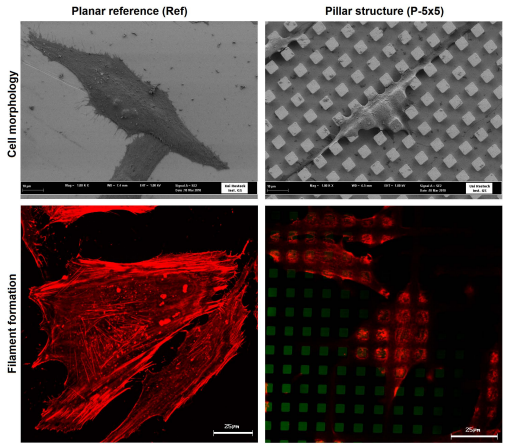


Jeschke et al. (2011): Exploring the performance of spatial stochastic simulation algorithms. J. Comput. Physics 230(7): 2562-2574 2011

Challenge II - The NOTORIOUS

Quantification of spatial data

- If we are interested in spatial phenomena, how do we quantify these data?
- Or are we satisfied with some face validation and that it somehow looks similar?



Bittig A.T., Matschegewski C., Nebe J.B., Stählke S. and Uhrmacher A.M.: Membrane related dynamics and the formation of actin in cells growing on micro-topographies: a spatial computational model. BMC Systems Biology, 2014

Challenge III - The GLORIOUS

"`Suitable"' languages for these systems

- Are very expressive spatial languages, extended non-spatial languages, or rather multi-formalism approaches the way to go?
- And BTW: what does suitable mean anyway?
- Can we "'quantify"' the value of a language, or will only the future tell us?

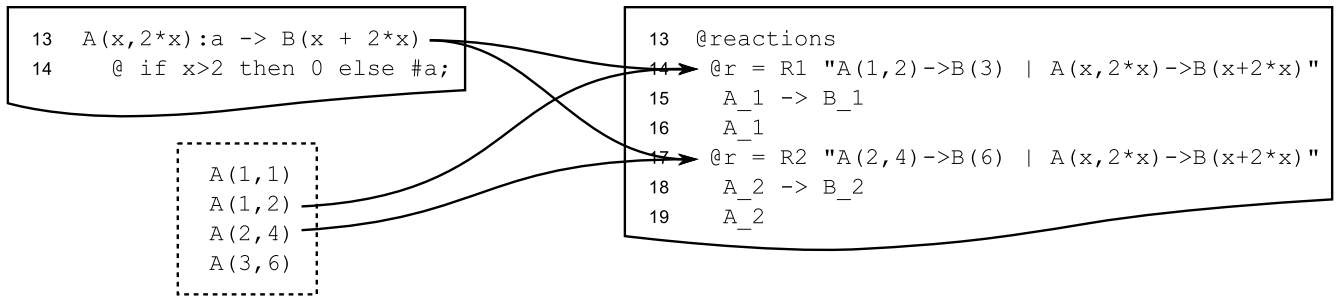
$$
\begin{array}{lcll}
C(v,p)[s?] & \rightarrow & C(v+(1/Td),p)[s?] & @\ \mathit{if}\ (p \in \{G1, SG2\})\ \mathit{then}\ k_6\ \mathit{else}\ 0 \\
C(v,G1)[s?] & \rightarrow & C(v,SG2)[s?] & @\ \mathit{if}\ (\mathit{count}(Mi,s?) > T7)\ \mathit{then}\ k_7\ \mathit{else}\ 0 \\
C(v,SG2)[s?] & \rightarrow & C(v,M)[s?] & @\ \mathit{if}\ (\mathit{count}(Ma,s?) > T8)\ \mathit{then}\ k_8\ \mathit{else}\ 0 \\
C(v,M)[s?] & \rightarrow & C(v/2,G1)[\mathit{fill}(l)] + C(v/2,G1)[\mathit{fill}(r)] & \\
 & & & @\ \mathit{if}\ (\mathit{count}(Ma,s?) < T9)\ \mathit{then}\ k_9\ \mathit{else}\ 0 \\
 & & & \quad \mathit{where}\ (l,r) = \mathit{half}(s?)
\end{array}
$$

Warnke T. et al. (2015): A Multi-Level Modeling Language for Simulating Cell Biological Systems. Proc. of PADS '15.

Challenge IV - The INFAMOUS

Ensuring reproducibility and reuse

- Spatial simulation tools are typically handcrafted, how can models run in one tool be run in another ensuring the same results?
- Different efforts to extend SBML seem hardly to converge, how can we succeed in spite of more complex models (e.g., the current whole cell initiative)?



Nähring S et al. (2013): From Standardized Modeling Formats to Modeling Languages and back - An Exploration based on SBML and ML-Rules. Proc. of WSC '13.

Lets get started!