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

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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?

\[ \text{NSM} \quad \text{Yes} \quad \text{if} \quad P \leq 10^4 \quad L \leq 11^3 \quad \text{No} \quad \text{NSM} \quad \text{Yes} \quad \text{if} \quad P \leq 272.7 \quad \text{No} \quad \text{NSM} \quad \text{Yes} \quad \text{if} \quad D \leq 4 \quad \text{No} \quad S^\tau (10) \]

\[ \text{NSM} \quad \text{Yes} \quad \text{if} \quad P \leq 10^6 \quad \text{No} \quad \text{NSM} \quad \text{Yes} \quad \text{if} \quad S^\tau (33) \quad \text{No} \quad \text{NSM} \quad \text{Yes} \quad \text{if} \quad D \leq 4 \quad \text{No} \quad S^\tau (10) \]

\[ \hat{P} : \text{Max. initial num. of particles per SV.} \quad L : \text{Num. of sub-volumes.} \]

\[ \hat{P} : \text{Avg. initial num. of particles.} \quad \hat{D} : \text{Max. diffusion rate.} \]

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?

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?

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

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)?

Let's get started!