

## **Title: Snapshot of reaction-diffusion simulations tools in neuroscience research**

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### **Abstract**

Advancements in computing power and cellular biology have allowed the development of various algorithms to simulate and analyse biological reaction-diffusion systems. With different algorithms and cell-level simulations tools available, evaluation and comparison of the systems' performance is important. This study aims to provide a snapshot of reaction-diffusion and co-simulation tools, including NEURON (Carnevale & Hines, 2006), ASTRO (Savtchenko et al., 2018), and NeuroRD (Oliveira et al., 2010), to determine their suitability for our research needs.

Here, we implement identical diffusion, reaction, and reaction-diffusion models with the selected tools and morphologies. We aim to assess the usability and stability of each tool, as well as the consistency of the results across them.

Our results highlight significant variability in the different tools. For example, some tools were not suitable for performing simulations with a realistic cell morphology, in which the use of more simplified geometries such as cylinders were justified. Additionally, variations in the computational efficiency and ease of implementation were observed, indicating trade-offs between flexibility, accuracy, and usability across the tools. However, despite the differences in the functionality, the simulation results revealed a high degree of similarity and consistent outcomes for the reaction-diffusion simulations.

When working towards more advanced and biologically accurate models, a thorough understanding of the capabilities and limitations of different tools is crucial. The expertise in the use of such tools enables the integration of multiple simulation approaches to broaden computational neuroscience research, with applications in personalized medicine and subject-specific analysis across healthy and disease conditions.