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Agent-based modelling of higher order chemical reactions using Smoluchowski kinetics

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Chemical reactions are traditionally modelled using deterministic methods such as ordinary differential equations. In biology, we also consider the effect of diffusion upon a reactive system. For small biological systems, it is necessary to use stochastic models. In this talk, we choose to use an agent-based model commonly known as Smoluchowski kinetics.

In the Smoluchowski model, two molecules diffuse in space, and react when they are within a critical separation distance (Smoluchowski radius). This radius is at a rate proportional to the reaction rate constant. Over the last 100 years, the model has been extended to incorporate reversible reactions by introducing a second separation distance.

A common problem with Smoluchowski kinetics is when modelling rapid enzyme reactions, where the assumptions used to model Smoluchowski kinetics break down. Using differential equations, these rapid interactions can be easily analysed using a pseudo steady state approximation which effectively results in non-linear reactions. Other models have utilised multiple timescales to model what is called fast-slow reaction kinetics.

In this talk, we theorise that a way to bypass the fast-slow reaction kinetics problem is to extend the Smoluchowski model to reversible trimolecular reactions. We develop these kinetics and apply them to the canonical Wnt signalling pathway. We model this pathway using traditional Smoluchowski kinetics, and show how the aforementioned issues come into effect. We then compare this to our trimolecular model and show how the issues disappear.

Primary author: CAVALLO, James (Monash University)

Co-author: Dr FLEGG, Mark (Monash University)

Presenter: CAVALLO, James (Monash University)

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