Discrete reaction-diffusion models

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Many processes in Chemistry and Biology involve the interplay between diffusion and reaction. Reactions depend on the local concentrations of the active species and have the effect of magnifying any concentration differences within the system. Diffusion attempts to spread out concentration gradients and the combination of these two effects can lead to propagating waves or patterns (steady, spatially nonhomogeneous structures) and to more complex behaviour, including spatiotemporal chaos. These systems are usually modelled by coupled reaction-diffusion equations which have the underlying assumption that the medium is a continuum, i.e. composed of an extremely large number of particles (molecules, cells) of a size that is very small compared to any external length scales.

This is a very good approximation for most chemical systems but is not so viable for some biological systems, where the number of cells, though large, is not suficiently so for the continuum approximation to hold. Also, there are some recent developments in chemical systems, microreactors and reactions within droplets in emulsions, where the continuum approximation can break down. These are referred to as being on the mesoscopic scale, lying between the microscopic (individual particles) and the macroscopic (continuum) scales. In these mesoscopic systems, 'diffusion' is modelled by an exchange process between neighbouring cells — 'discretized diffusion'. This turns the model from one involving (a few) partial differential equations into a large system of ordinary differential equations.

The project starts by looking at one particular mesoscopic system based on the Nagumo model for the propagation of signals along nerves following the paper by Erneux and Nicolis [1]. The discretized version can lead to propagation failure not seen in the continuum case. The aim is to extend this work to include the effects of transport caused, for example, by an external electric field (modelled simply). A further development could include applying the ideas gained from the simple model to systems with more complicated (excitable) kinetics as these can be more realistic models of biological systems. The project will mainly involve both numerical simulations and asymptotic analysis (perturbation theory) based on small parameters that arise in the system.

1. T. Erneux, G. Nicolis. Propagating waves in discrete bistable reaction-diffusion systems. *Physica D* **67**, (1993) 237–244.