Dynamical Systems with Python - Workshop 1: An Introduction to Dynamic Modelling - Building a Model

We start with reactions in time and end with dynamics in time and space.

1. Michaelis Menten (MM) and Hill kinetics in the steady state. MM is nonlinear but expected. Hill with n>1 is nonlinear with a qualitative transition. Predict 0 -> 1 sigmoidal changes in open flow. Open flow and nonlinearity are the basic ingredients of every complex living systems. Type the model and run it. Mathematics: nonlinear functions.

2. Forward inhibition induces a new feature, namely, instability. The lower and the upper state of the Hill function can now overlap and co-exist. Example: ATP kinetics of the PFK1 reaction. This allows switching between states by external regulatory processes. Mathematics: Bifurcations.

3. Extensions: Additional feedback inhibition leads to spontaneous oscillations and self-organised temporal order. Processes can switch autonomously and repeatedly. Adding features can increase the complexity of self organisation, the idea of a hierarchy.

4. In space a grid is needed to describe what happens at each location. Diffusion is the simplest processes to mediate spatial coupling: a material flow happens whenever there is a gradient between neighbouring grid points. Diffusion itself is passive and attempts to homogenise but with nonlinear kinetics leads to patterns that (self-)organise time and space. Incredibly rich dynamics is possible in space. Transitions can be normal or abnormal. Data analysis and perturbation experiments help to figure out key components of phenomena.

Nonlinear Enzyme Kinetics:

1. Hill equation with special case n=1
2. Brief analysis of functions
3. Rate landscape

Focus: physical chemistry

Bistability:

1. Reaction scheme(s)
2. Time Series: two fates
3. Bifurcation diagram
4. Steady State and Potential Analysis
5. Waddington Potential Landscape

Focus: Programming

Oscillations:

1. Reaction scheme(s)
2. Time Series: SS or LC
3. Bifurcation diagram:
4. State Space Analysis
5. Animated oscillations

Focus: systems theory

Spatiotemporal Waves:

1. Diffusion only Animation
2. Reaction CICR 2V model
3. CICR in a 2D reaction-diffusion medium: spontaneous & with stimulation

Focus: connection with experiment

Some Experimental Findings:

Cardiac spiral waves: https://www.teledynevisionsolutions.com/en-gb/learn/learning-center/scientific-imaging/whole-tissue-calcium-imaging/

Calcium waves in hippocampus slices: https://journals.physiology.org/doi/full/10.1152/jn.1998.79.2.1045

Calcium waves in development (gastrulation) https://www.pnas.org/doi/10.1073/pnas.96.1.157#supplementary-materials

Video: Calcium waves in epithelial cells: