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| 1 | Edward | Acheampong | Mathematical modelling to explore pharmaceutical drug processing in wastewater treatment | |
| 2 | Mayte | Bonilla Quintana | An integrate-and-fire network model for grid cell dynamics | <p>In 2005, Hafting et al. at the Moser Lab, discovered grid cells in the Medial Entorhinal Cortex (MEC). These cells fire at multiple locations while an animal is wondering through an environment defining a periodic triangular array that covers the entire surface, hence the name. Furthermore, grid cells fire at the same position regardless of changes in the animal's speed and direction, and firing persists in the absence of visual input. It is therefore believed to correspond to the animal's own sense of location. For the discovery of these type of cells May-Britt and Edvard Moser won the 2014 Nobel Prize in Physiology or Medicine.</p> <p>Since the discovery of grid cells many models have been developed in order to address the mechanism of grid cell firing. However only few models link the firing of grid cells to data on intracellular resonance and rebound spiking in layer II stellate cells of the MEC, that represent the 70% of the total MEC II neural population and therefore a large fraction of the grid cell population.</p> <p>We propose a neural field integrate and fire model with a hyperpolarisation activated cation current (h-current). The model is motivated by previous ones in which wave generation in spiking neural networks is hypothesised to underly the formation of grid cell firing fields but within a framework that allows for analytical tractability. Furthermore, inspired by relevant MEC data we consider only inhibitory neural connectivity. Simulations of our model show sustained rebound spiking that is propagated across the network after injecting a initial hyperpolarising current to a small fraction of the neurons.</p> <p>Our aim is to show that a difference in the h-current time constant seen experimentally along the dorsal to ventral axis of the MEC can produce a difference in the size and spacing between the grid cell firing fields. In order to achieve this, we first perform a piece-wise linear reduction of our model that preserves its dynamics. Such a reduction allows us to obtain a self-consistent solution for a periodic travelling wave. We developed a wave stability analysis using theory of non-smooth systems and observed a strong dependence of the period on the h-current time constant.</p> |

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| 3 | Lee | Curtin | Homogenisation of Diffusion Applied to a Novel Chemotherapy Drug Delivery System | |
| 4 | Joshua | Davis | Travelling wave and bump dynamics in a spiking neuronal network | <p>As a result of modern imaging technologies, waves and bumps of neuronal activity have been experimentally verified at a variety of spatial scales in the cortex. Spatially localised bumps of activity are known to be involved in mechanisms of orientation tuning in the visual cortex, the rat head direction system, and working memory. In the turtle visual cortex, the presentation of stimuli has been shown to evoke propagating waves of neuronal activity. Numerous mental processes including sleep and binocular rivalry are characterised through waves, as well as neurological disorders such as epilepsy and migraines.</p> <p>Simulations of a discrete spiking network of integrate-and-fire network are shown to exhibit a rich variety of bump and wave states. In particular we find a family of coherent pulsating wave states composed of multiple, synchronously firing neurons in a localised region of the spatial domain. A continuum assumption is then taken to construct analytical solutions of such waves solely in terms the mean wave speed and firing times. The stability of the multiple spike waves is analysed by perturbing around the firing times and an eigenvalue problem is solved and tested in the discrete regime. Numerical continuation is used to gain insight into the bifurcation structure of such waves investigated in terms of the parameters governing synaptic efficacy and connectivity. It is shown that multiple spike waves destabilise via a sequence of Hopf bifurcations. In addition, composite wave solutions are also found that match up in simulation to multiple spike pulses that have combined and coalesced.</p> |
| 5 | Etienne | Farcot | A Modular Analysis of the Auxin Signalling Network | <p>Auxin is essential for plant development from embryogenesis onwards. Auxin acts in large part through regulation of transcription. The proteins acting in the signalling pathway regulating transcription downstream of auxin have been identified as well as the interactions between these proteins, thus identifying the topology of this network implicating 54 Auxin Response Factor (ARF) and Aux/IAA (IAA) transcriptional regulators. Here, we consider a mathematical model of this pathway, focusing on the role played by five functional modules into which the auxin pathway can be decomposed: the sequestration of ARF by IAA, the transcriptional repression by IAA, the dimer formation amongst ARFs and IAAs, the feedback loop on IAA and the auxin induced degradation of IAA proteins. Focusing on these modules allows assessing</p> |

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| | | | | <p>their function within the dynamics of auxin signalling. One key outcome of this analysis is that there are both specific and overlapping functions between all the major modules of the signalling pathway. This suggests a combinatorial function of the modules in optimizing the speed and amplitude of auxin-induced transcription. Our work allows to identify potential functions for dimerization of transcriptional regulators on the amplitude, speed and sensitivity of the response and a synergistic effect of the interaction of IAA with transcriptional repressors on these characteristics of the signalling pathway.</p> |
| 6 | Michael | Forrester | Structure-Function Clustering in Multiplex Brain Networks | <p>The relation between the human brain's anatomical structure and its emergent function is yet poorly understood. Extending standard metrics from the field of graph theory, we study this relationship in a network of coupled Wilson-Cowan oscillators to show that synchronous activity is influenced by structural connectivity.</p> |
| 7 | Aytol | Gokce | Reduced dynamics of pattern formation in a planar neural field model | |
| 8 | Chris | Lanyon | Should we worry about slurry? | |
| 9 | Jakub | Kory | TBC | |
| 10 | | MASS Cohort 2 | Fuel for Thought: Driving Towards a Proposed Hydrogen Infrastructure for Nottingham. | |
| 11 | Chris | Miles | Phase-Field Model for Surface Coverage of Thin Films | <p>We propose a non-linear PDE model describing surface coverage of thin films deposited onto a substrate. The equations are derived from energy minimisation using phase-field modelling techniques. This is an important consideration in fabricating efficient thin film solar cells. The model is discretized using finite elements and a third order IMEX Runge-Kutta method and used to simulate post-deposition morphological changes.</p> |

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| 12 | Peer-Olaf | Siebers | Facilitating Multidisciplinary Agent-Based Social Simulation Modelling: A (More) Formal Approach | <p>When aiming to develop Agent-Based Social Simulation (ABSS) models one faces the question of how to build them and where to start. This can be challenging not only for novices in the field but also for multidisciplinary teams where it is often difficult to engage everyone in the modelling process. In this case co-creation is an important aspect. Team members need to be open minded about the use of new tools and methods and about the collaboration with researchers from other domains and business partners.</p> <p>Over the years we have developed a quite sophisticated "plan of attack" in form of a framework that guides the model development. The EABSS (short for Engineering ABSS) framework supports model reproducibility through rigorous documentation of the conceptual ideas, underlying assumptions and the actual model content. It provides a step-by-step guide to conceptualising and designing ABSS models with the support of Software Engineering tools and techniques. While this framework will not work perfectly for all possible cases, it provides at least some form of systematic approach. The user should be prepared to adapt it to fit individual needs.</p> |
| 13 | Agne | Tilunaite | Cellular calcium signalling in the presence of single cell variability and dynamic stimuli | <p>Under physiological conditions, cells often experience time dependent stimuli such as transient changes in neurotransmitter or hormone concentrations, but it remains an open question how cells transduce such dynamic stimuli. We exposed HEK293 cells and astrocytes to dynamically varying time courses of carbachol and ATP, respectively, and investigated the corresponding cellular calcium spike sequences. While single cells generally fail to follow the applied stimulation due to their intrinsic stochasticity and heterogeneity, faithful signal reconstruction is observed at the population level. We provide a simple transfer function that explains how dynamic stimulation is encoded into ensemble calcium spike rates.</p> <p>When dynamically stimulated, different cells often experience diverse stimuli time courses. Furthermore, cell populations may differ in the number of cells or exhibit various spatial distributions. In order to understand how these conditions affect population responses, we compute the single cell response to a given dynamic stimulus. Single cell variability and the small number of calcium spikes per cell pose a significant modelling challenge, but we demonstrate that Gaussian processes can successfully describe calcium spike rates in these circumstances and outperform standard tools such as peri-stimulus time histograms and kernel smoothing. Having the single cell response model will allow us to compare responses of various sets of</p> |

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| | | | | cells to the observed population response and consequently obtain insight into tissue-wide calcium oscillations for heterogeneous cell populations. |
| 14 | Tim | Whiteley | Modelling urban population dynamics using coupled integro-differential equations | Current urban population models do not explain how population distributes within a city or the expected locations of growth and decay over longer time periods. This research seeks to identify key factors which determine such urban population distributions by using an integro-differential equation model to simulate population change in symbiosis with service provision. The assumption is that people and services benefit from close proximity but only where there is space available. This system may tend towards a spatially homogeneous distribution or a spatial pattern. Using Gaussian spatial weight kernels, linear stability analysis performed at the spatially homogeneous steady state shows that stability depends on a key function; the carrying capacity for services given a local population density. In particular, instability can only occur where the carrying capacity function is convex with respect to population density. Furthermore, this spatial instability can occur only for perturbations with a sufficiently long lengthscale. The analysis may explain how the spatial and local interactions between populations and services can drive the emergence of patterns in cities, and could predict the characteristic scale of such patterns. |