Abstracts of Posters

Modelling ion channels with Brownian Dynamics

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Ion transport across cell membranes plays a fundamental role in human, animal and bacterial cells. Of the many computational methods used to investigate ion channels, Brownian Dynamics (BD) is of particular importance. This models ions in a water-filled charged protein using the over-damped Langevin equation due to the low Reynolds number of the ions. It is an electrostatic system and so, to ensure self-consistency the system must be coupled to the Poisson equation, which must be solved at fixed time steps to build a picture of each ions' trajectory.

The model (Kaufman et al 2013a) has proven successful at modelling the flow of ions in Ca^{2+} and Na^{+} channels and replicating key features such as selectivity and anomalous mole fraction effect (AMFE). It has been shown that Ca^{2+} and Na^{+} channels have distinct conduction and occupation bands as a function of the channel's charge. Further investigation of these bands has led to two important conclusions. First, consideration of the energetics in the system suggests that these bands correspond to a phenomenon known as barrier-less conduction (Berneche 2001, Yesylevskyy 2005). Secondly these bands can be thought of as ionic Coulomb Blockade (CB) analogous to electron CB as seen in a quantum dot. (Kaufman et al 2013a, Kaufman et al 2013b, Kaufman et al preprint)

Ion channels can be treated mesoscopically therefore exhibiting quantum-like features. These include, the aforementioned ionic CB, but also the use of the Fermi-Dirac distribution for occupation and the possibility of discussing ionic dynamics via a Schrödinger-like wave equation (Kamenev 2006). These features will be discussed.

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Layered architecture shapes context-dependent response and input integration of a cortical circuit

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Lamination is a landmark feature of cortical architecture. But even if functional specializations of individual layers have been suggested (Raizada and Grossberg 2003; Hirsch and Martinez 2006), the role played by interlayer connections in shaping the dynamical responses of a cortical column has not yet been fully elucidated.

Here, we analyze a mean-field model of a cortical column, embedding realistic interlayer connections (the one-column "connectome" of Binzegger et al. 2004). Systematically varying efficacy of excitation and inhibition in the model we find phase diagrams showing a great diversity of possible dynamical regimes. In particular, due to the presence of delayed inhibition, oscillations can be generated. Oscillations in different layers may be phase-locked or phase-precessing and have different frequencies. In some regions of the phase diagrams high frequencies (gamma-like) predominate in L23 while low beta-like frequencies predominate in L5. Remarkably, while this experimentally observed tendency is usually attributed to the different cortical sources to different layers, here it arises spontaneously in an isolated model column, resulting from the multilayer connectivity. The column is thus intrinsically predisposed to communication-through-coherence processes over multiple frequency bands. Furthermore, we find that horizontal or top-down currents, mediating perceptual context information, are non-linearly amplified and that vertical inter-layer interactions alone already contribute to contextual modulations of the column response, besides other interactions here not explicitly modeled. Our model predicts interlayer competition behaviors which could be probed experimentally by selective optogenetic (in)activation techniques. Finally, the robustness of our findings is discussed by comparison with alternative wiring diagrams.

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Chaotic behavior of R Scuti and R Leonis

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We shall present phase portrait reconstruction of two variable stars – R Scuti and R Leonis. The studied stars are at the end of their lifetimes (they burned all hydrogen in their cores). R Scu is RV Tauri type star, radially pulsating low mass supergiant; R Leo is a cool red giant (type Mira). Data for the analysis were obtained from the AAVSO database. Phase portraits were reconstructed using the method of time delayed coordinates. Proper time delays and the embedding dimensions were estimated from the first minimum of mutual information. From computed maximum Lyapunov exponent and correlation dimension was proven that R Scu star exhibits chaotic behavior and thus we confirmed results made by Buchler et al., who were using different method. In the case of R Leo star results are quite uncertain and we still cannot confirm underlying low-dimensional dynamics. We also found that noise can have a big influence on the results so we have to be carefull about choosing the right method for noise reduction. The TISEAN package was used for processing all the data.

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Can single cancer cell behaviour be related to local blood flow dynamics?

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Motivated by recent results in which the microvasculature local to malignant melanoma was found to exhibit reduced vasomotion when compared to that in healthy skin and atypical naevi [1], we seek to understand these results through the development of a cellular model of cancer, based on alterations to oscillations which are known to be present in healthy cells.

Previous studies have found oscillations in metabolism, both in the mitochondria [2] and during glycolysis [3], and one of their most crucial products, ATP. These oscillations in ATP have been related to oscillations in the cell membrane potential. Cancer cells are known to have suppressed mitochondria, possibly to prevent apoptosis, and upregulated glycolysis, to enhance survival probability during periods of hypoxia. Another universal feature of cancer cells is the depolarization of their cell membrane potential [4], which may be related to their being constantly in a state of proliferation.

We hypothesize that modelling the cell membrane potential of a cancer cell in terms of coupled cellular oscillators, and allowing for time-varying but stable frequencies using the recently developed class of non-autonomous systems known as chronotaxic systems [5, 6, 7], will allow us to link the behaviour of a single cancer cell to the macroscopic changes in blood flow observed in reality.

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Supply Networks: Instabilities without Overload

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Supply and transport networks support many biological processes and much of our technical infrastructure. Their reliable function is thus essential for all aspects of life. Transport processes involving quantities beyond the pure loads exhibit alternative collective dynamical behaviour compared to processes exclusively characterized by loads. Here we report that oscillator models describing electric power grids can exhibit instabilities even if there is no overload.

We first characterize the fixed points (normal operation of the grid) in the limit of zero dissipation in terms of Hamiltonian dynamics. In systems with dissipation, all fixed points are identical to local extrema/saddle points of the (Hamiltonian) potential, which depends on the network topology. We classify spectral and asymptotic stability properties of fixed points and provide an elementary example. We show using graph theoretic tools that if the phase difference along each transmission line $|\theta_j - \theta_i|$ is not more than $\frac{\pi}{2}$, then instability is always caused by an overload on one or more lines. However, if one or more lines have phase difference exceeding $\frac{\pi}{2}$, we demonstrate that a fixed point can lose stability even though no line is overloaded. This phenomenon may also emerge in other sufficiently complex supply or transport networks.

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Mathematical modeling of intracellular Ca^{2+} and membrane potential dynamics in the beta cell syncytium

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Pancreatic beta cells in the islets of Langerhans regulate whole body nutrient homeostasis by secreting the hormone insulin in a regulated manner. Glucose stimulation elicits depolarization of the cell membrane by decreasing the open probability of ATP sensitive K^+ ion channels, which results in electrical activity of beta cells in terms of Ca^{2+} entry and action potential firing. Ca^{2+} subsequently acts on the exocytotic machinery to stimulate fusion of insulin-containing vesicles with the plasma membrane for secretion into the bloodstream [MacDonald & Rorsman, 2006]. The bulk of evidence indicates that the Ca^{2+}, electrical and secretory responses of beta cells to glucose are not only properties of individual cells but also crucially rely on collective activity of cell populations [Rutter & Hodson, 2013]. However, the precise mechanisms of the nature and extent of coupling within the syncytium are poorly understood. A thorough understanding of all these complex molecular, cellular and intercellular mechanisms that govern the functioning of islets, requires the support of mathematical modeling of physiological data. Existing models for beta cells are generally based on the Hodgkin-Huxley equations for neuronal electrical activity, although many efforts have been made to incorporate cell-specific details as well as different aspects of intercellular communication [Hraha *et al.*, 2014]. Despite the fact that many of the established computational models fit well the various aspects of intra- and inter-cellular dynamics observed in previous experiments, they fail to firmly describe our novel and most recent experimental results obtained by means of in situ acute mouse pancreas tissue slice preparation with noninvasive fluorescent calcium and voltage labeling and the subsequent confocal laser scanning microscopy [Stožer *et al.*, 2013, Dolenšek *et al.*, 2013]. In order to address this issue we upgrade the existing modeling approaches and develop a detailed model of interconnected beta cells, which incorporates additional physiological specifics and leads to a better agreement between our experimental findings and theoretical predictions. Our results exemplify that a combination of modern high spatial and temporal resolution confocal imaging and computational modeling is a powerful approach that leads to a comprehensive understanding of the islet topology and its function.

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Probing the role of accelerator modes on the dynamical localization properties of the quantum kicked rotator and on the anomalous diffusion of its classical analogue

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We study the N-dimensional model of the quantum kicked rotator in the classically fully chaotic regime, which in the limit of sufficiently large N tends to the quantized kicked rotator. We describe the features of dynamical localization of chaotic eigenstates as a paradigm for other both time-periodic and time-independent (autonomous) fully chaotic or/and mixed type Hamilton systems. We generalize the scaling variable to the case of anomalous diffusion in the classical phase space, by deriving the localization length for the case of generalized classical diffusion. We then focus on the effect of the anomalous diffusion arising due to the accelerator modes in the classical kicked rotator, exemplified by the standard map. The systematic approach rests upon detecting the regular and chaotic regions and thus to describe in detail the structure of the phase space, the description of the momentum distribution in terms of the Lévy stable distributions, the numerical calculation of the diffusion exponent and of the corresponding diffusion constant. We use this approach to analyze in detail and systematically the standard map at all values of the kick parameter K, up to $K = 70$. All complex features of the anomalous diffusion are well understood in terms of the role of the accelerator modes, mainly of period 1 at large $K \geq 2\pi$, but also of higher periods (2,3,4,...) at smaller values of $K \leq 2\pi$.

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MATHEMATICAL MODELING OF PLANAR CELL POLARITY IN EPITHELIAL TISSUES DURING DEVELOPMENT

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Abstract

The polarization of epithelial cells in the plane of a tissue is referred to as planar cell polarity (PCP) and is of crucial importance for the normal development of specialized biological structures and hence a biological organism as a whole. The term polarity in PCP is related to the asymmetric distribution of core PCP proteins involved in the intra-cellular signaling pathway [1]. Experimental studies performed on the wings of the Drosophilia fly have shown that PCP of individual cells is established through the interplay between intra- and inter-cellular communication accompanied by a global cue. Although most of the existing knowledge on PCP is based on experimental studies done on fly wings, the same mechanism have been found to govern the establishment of PCP in vertebrates [2]. Faults in PCP signaling caused by mutations in the intra-cellular signalization lead to impaired polarity patterns of the epithelium layer, which can result in serious pathological conditions [3]. Computational modelling have proven to be a very reliable approach for studying the complex processes involved in PCP. The strategy of in silico experiments enables a precise tracking of the behavior and spatial arrangement in case of different dysfunctions in intra-cellular signaling. In our previous study [4], we constructed a mathematical model of the epithelium mono-layer as a 2D hexagonal grid, where each hexagon in the lattice represents an epithelial cell. The modeling of the orientation and magnitude of polarization of individual cells and the intercellular interactions is based on the theoretical framework introduced by *Hazelwood&Hancock* [5]. The model includes only physically relevant terms that account for the cells ability to maintain its own intracellular polarisation, interact with the polarity of adjoining cells and interact with a global field, which are described by a free energy function. The stationary polarity patterns are acquired by numerically integrating the free energy function and finding its global minima. Here we extend our previous studies to non-uniform cell shapes and consequently a varying number of neighbouring cells. The increased heterogeneity in the shape of the cells is also implemented in the free energy function by weighting inter-cellular interactions in accordance with the length of tight junctions between two cells. We investigate the role of cells with impaired intracellular signalling, i.e. mutant cells, on the global pattern formation. For the characterization of the polarized cytoarchitectures we use the local and global order parameters. We additionally analyse the possible scenarios of PCP establishment during development, with emphasis on the impact of mutant cells on the overall organization in the global polarity pattern.

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On-off intermittency generated by infinite-modal maps

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On-off intermittency is an irregular switching phenomenon between long-term laminar behavior and instantaneous bursts. This phenomenon was discovered by Fujisaka and Yamada [1] in coupled chaotic systems, and observed in many experimental systems or mathematical models. Conventional mathematical models for on-off intermittency have been modeled using linear multiplicative noise systems. In such systems, it has been found that statistical properties such as the following are true at near the transition to transient behaviors from intermittent behaviors: (i) The stationary distribution about the distance r from the laminar state has $P(r) \sim r^{-1}$ $(r \ll 1)$ [2], (ii) The laminar duration distribution has $\rho(t) \sim t^{-3/2}$ $(t \gg 1)$ [3]. Since the above laws was observed from many experimental systems as well as mathematical models, they are regarded as the standard statistical laws for on-off intermittency.

Recently, in response to experimental examples deviating from such standard statistical laws, a probabilistic model which can change the exponents, such as -1 or $-3/2$, of the standard statistical laws by control parameters is devised [4]. However the deterministic model generating the non-standard statistical laws is not yet known. In such a situation, we found that the following one-dimensional dynamical system, which is an infinite-modal map, can generate on-off intermittency chaos:

$$x_{n+1} = x_n |x_n|^{a-1} \sin\left(b \log\left(1/|x_n|\right)\right), \quad -1 \le x_n \le 1. \tag{1}$$

where $a \in (0,1)$ and $b > 0$ are parameters. This map originates in the dynamics for near the homoclinic orbit of the saddle-focus point in ordinary differential equations [5,6]. In this presentation, we present that the essence for the dynamics of this map is a non-linear multiplicative noise system and that it has non-standard statistical laws, according to numerical simulations.

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THE GRAVITATIONAL BILLIARD

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This paper concerns the motion of a point particle moving in a symmetric wedge of angle 2α subject to a constant gravitational field of magnitude g, pointing downward along the direction of the axis of symmetry. All collisions are assumed to be elastic, thus total mechanical energy is conserved. This system is a rather simple one, that shows a remarkable complex behavior in spite of its two degrees of freedom. Since its main properties are already known (e.g. KAM regions, Lyapunov exponents etc.), the aim of this paper is to show a different way to approach the problem, using cartesian coordinates instead of polar. The region of integrability ($\alpha = 45°$) will be the one of main interest; a new constant of motion at $\alpha = 45°$ will be found and used as a tool to observe a chaotic attractor-like behavior just outside the region of integrability.

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Swarm Dynamics and Lyapunov Analysis

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The swarm dynamics is characterized by many local and global modes in the collective motions. The global response in the group dynamics is sensitively affected by the local aspects and also the local behaviors are controlled by the global information. The local-global linkage in the swarm dynamics is an essential mechanism, which leads to self-organization of the unified behavior in the swarm dynamics. In this paper, we consider a simple model to understand the linkage between local and global effects in the group dynamics by taking into account the local communicative interactions as well as the global environmental effects.

We propose the minimal model of active matters, where two parameters play the essential role in the group behavior: one is the environmental effect from the outside of the swarm, and the other is the communicative effect among individuals inside of swarm. The velocity of the i-matter is described by the following dynamics;

$$\dot{\mathbf{v}}_i(t) = \left(1 - |\mathbf{v}_i(t)|^2\right) \mathbf{v}_i(t) + \mathbf{F}^{comm}(t) + \mathbf{F}^{goal}(t) + \mathbf{F}^{env}(t) \tag{2}$$

For the sake of simplicity, the attractive effect of the goal information is shown by $\mathbf{F}^{goal}(t)$, the environmental effect from outside by $\mathbf{F}^{env}(t)$, and the communicative competence among individuals by $\mathbf{F}^{comm}(t)$. The first term is also a simplified form of the self-controlling effect to each velocity.

The Lyapunov exponents, which describe the sensitivity in the motion of each individual, is used to understand the global and local behaviors of the swarm dynamics. Increasing the size of the swarm, the exponents also increase. It will be discussed that the Lyapunov exponents (spectrum) affect the swarm dynamics of our model sensitively and the relation between the collective states and the instability. Detailed aspects of the Lyapunov exponents in the swarm dynamics are discussed in comparison with other chaotic dynamics of many-body systems.

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THE STUDY OF HURST EXPONENT OF KEPLER CONTACT BINARIES

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We have measured the Hurst Exponent (HE) of 19 (up to now) Center Between Maxima (CBM) O-C diagrams of contact binaries observed with the Kepler space telescope, developed for following the migration of star spots with high precision. All of the HEs are significantly greater than 0.5, indicating a persistent behavior. One of the binaries (KIC 6057829) posseses an HE close to unity, implying strict periodicity underlying the fluctuating migration, confirmed by the Lomb-Scargle periodogram. The correlation between HE and orbital period shows that high HE (¿0.9) binaries tend to gather around a typical contact binary period (0.37 day). The correlation between HE and the spot activity period shows a considerably uniform distribution among all HE values. The ongoing research may provide significant insight in the spot migration dynamics in the near future.

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CHARACTERIZING COUPLING FUNCTIONS IN NETWORKS OF OSCILLATORS

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Networks can be found everywhere in nature: from large-scale climatic interactions, to medium-scale synchronously firing ensembles of neurons in the brain, to small-scale coupled molecular systems. How to characterize and reconstruct networks from data is therefore a challenge which pervades all of science.

Numerous methods that detect the existence of causal connections in networks have already been introduced. However, they are mainly focused to pairwise interactions.

Here we present a new method, based on dynamic Bayesian inference which is capable to detecting effective phase connectivity between networks of time-evolving coupled oscillators subject to noise.

As we will see, it can reconstruct not only pairwise, but also joint and higher degree conductivities, including triplets and quadruplets of interacting oscillators.

Moreover, one can infer details of coupling functions from which the existence of causal links can be determined as well as the underlying functional mechanisms.

We will illustrate the characteristics and potentials of the method using an example of numerically generated network of phase oscillators with time-dependent coupling parameters and subject to noise. Furthermore, results from real data with extracted coupling functions between EEG brain waves will be shown.

The coupling functions of the pairwise $\delta - \alpha$ interactions and the triplet $\theta - \alpha - \gamma$, including their functional forms, will be presented in detail. Based on multi-channel recordings, spatial connectivity between these brain waves will also be revealed, thus illustrating the great potentials of our new method for reconstructing properties of networks of interacting oscillators in general.

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