2013-14 Warwick EPSRC Symposium on Statistical Mechanics

Models from Statistical Mechanics in Applied Sciences

University of Warwick, 9-13 September 2013

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Abstracts

Tibor Antal *Modeling cancer as a stochastic process*

Stochasticity is essential when modeling initiation of tumors, progression of tumors from benign to malignant states, or metastasis formation. Many aspects of these phenomena can be modeled by simple multi-type branching processes, and the results compare fairly well with experimental and clinical data. These models then can be used to optimize drug treatments. Spatial heterogeneity of tumors is also important for treatment, and their exploration has recently begun by modeling the interplay between tumor shapes and genetic mutations.

Cecile Appert-Rolland *Exclusion processes and pedestrians*

It is known that some diagonal patterns form spontaneously at the crossing of two perpendicular pedestrian flows. Here the system is modeled by multiple exclusion processes. We find that the pattern is not purely diagonal but has slightly the shape of chevrons. We provide an analysis for this pattern formation, based first on a macroscopic mean-field approach and second on a microscopic calculation of effective interaction. The connection with bath-mediated interactions in colloidal systems will be discussed.

References:
[1] J. Cividini, C. A-R, and H.J.Hilhorst, Europhysics Letters 102 (2013) 20002
[2] arXiv:1305.7158
[3] arXiv:1305.3206

Baruch Barzel *Universality in Network Dynamics*

Despite significant advances in characterizing the structural properties of complex networks, a mathematical framework that uncovers the universal properties of the interplay between the topology and the dynamics of complex systems continues to elude us. This challenge requires us to connect the microscopic dynamical rules governing the pairwise interactions with the macroscopic observations of the system's behavior. Answering questions such as how the spread of influence differs from social interactions to biochemical or genetic regulation, or which nodes have the strongest influence in different systems. To address these questions we adopt a statistical mechanics approach and focus on a complex system's response to external perturbations, capturing its inherent flow of information and influence. We find that we can predict a set of pertinent characteristics directly from the dynamical equations describing the system's interactions. The result is a unified framework that can treat diverse dynamical systems, uncovering their deep universality of dynamical behavior. Hence while complex systems are characterized by extreme microscopic diversity their macroscopic behavior is restricted to a discrete set of permitted dynamical behaviors, insensitive to specific microscopic details. Finally, we examine the inverse process: reverse engineering the dynamical equations that govern the system from macroscopic external observations. Namely we attempt penetrate the black box of complex systems, analytically peeking into the dynamical mechanisms of their pairwise interactions.

Ginestra Bianconi *Dynamics, Entropy and Information in Temporal Social Networks*

The recent availability of data describing social networks is changing our understanding of the ”microscopic structure” of a social tie. A social tie indeed is an aggregated outcome of many social interactions such as face-to-face conversations or phone calls. Analysis of data on face-to-face interactions and phone-calls shows that such events are characterized by heterogeneous duration of contacts, which can either follow a power-law distribution, such as in face-to-face interactions, or a Weibull distribution, such as in mobile-phone communication. In this talk we present a model for social interactions at short time scales, based on a reinforcement dynamics. In this model the longer two individuals interact the smaller is the probability that they end their conversation. We quantify the information encoded in the dynamics of these networks by the entropy of temporal networks. Finally, we show evidence that human dynamics is able to modulate the information present in social network dynamics when it follows circadian rhythms and when it is interfacing with a new technology such as the mobile-phone communication technology.

Richard Blythe
Spatiotemporally complete condensation in a non-Poissonian exclusion process

We investigate a non-Poissonian version of the asymmetric simple exclusion process, motivated by the observation that motor proteins hop as a consequence of some internal dynamics which yields a non-Markovian (history-dependent) hopping process. We characterize a large family of processes using a waiting-time distribution for individual particle hops. We find that when the variance of this distribution is infinite, a real-space condensate forms that is complete in space (involves all particles) and time (exists at almost any given instant) in the thermodynamic limit. The mechanism for the onset and stability of the condensate are both rather subtle, and depends on how the microscopic dynamics subsequent to a failed particle hop attempt are defined.

Freddy Bouchet *Phase transitions and large deviations in geophysical fluid dynamics*

Geophysical turbulent flows (atmosphere and climate dynamics, the Earth core dynamics) often undergo very rapid transitions. Those abrupt transitions change drastically the nature of the flow and are of paramount importance, for instance in climate. By contrast with most theoretical models of phase transitions, for turbulent flows it is difficult to characterize clearly the attractors (they are not simple fixed points of a deterministic dynamics or statistical equilibrium states) and the trajectories that lead to transitions from one attractor to the others.

I will review recent researches in this subject, including experimental and numerical studies of turbulent flows. Most of the talk will focus on theoretical works in the framework of the 2D stochastic quasi-geostrophic Navier-Stokes equations, the quasi-geostrophic equations, and the stochastic Vlasov equations. We will discuss predictions of phase transitions, validity of large deviation results of the Freidlin-Wentzell type, or more involved approaches when the Freidlin-Wentzell approach is not valid.

The results involve several works that have been done in collaborations with J. Laurie, M. Mathur, C. Nardini, E. Simonnet, J. Sommeria, T. Tangarife, H. Touchette, and O. Zaboronski.

Tiziana di Matteo
New tools in statistical mechanics to detect information in financial datasets

In complex datasets information is often hidden by a large degree of redundancy and grouping the data into clusters of elements with similar features is essential in order to reduce complexity. However, the reduction of the system into a set of separated local communities may hide properties associated with the global organization. It is therefore essential to detect clusters together with the different hierarchical gatherings above and below the cluster levels. In this talk I will introduce a graph-theoretic approach to extract clusters and hierarchies in an unsupervised and deterministic manner, without the use of any prior information [1,2]. I will show that applications to financial data-sets can meaningfully identify industrial activities and structural market changes. I will also discuss a new technique by means of filtered graphs [3,4] to diversify financial risk and I will show how this approach can be used to build a well-diversified portfolio that effectively reduces investment risk. Specifically I will show that investments in stocks that occupy peripheral, poorly connected regions in the financial filtered networks are most successful in diversifying investments even for small baskets of stocks. On the contrary, investments in subsets of central, highly connected stocks are characterized by greater risk and worse performance [5].

References:
[1] Won-Min Song, T. Di Matteo, T. Aste, "Nested Hierarchy in planar graphs", Discrete Applied Mathematics 159 (2011) 2135.
[2] Won-Min Song, T. Di Matteo, T. Aste, "Hierarchical information clustering by means of topologically embedded graphs", PLoS One 7(3) (2012) e31929.
[3] T. Aste, T. Di Matteo, S. T. Hyde, "Complex networks on hyperbolic surfaces", Physica A 346 (2005) 20-26.
[4] M. Tumminello, T. Aste, T. Di Matteo, R. N. Mantegna, "A tool for filtering information in complex systems", PNAS 102, n. 30 (2005) 10421.
[5] F. Pozzi, T. Di Matteo and T. Aste, "Spread of risk across financial markets: better to invest in the peripheries", Scientific Reports 3 (2013) 1665.

Eric Vanden-Eijnden *A tour on the computational side of large deviation theory*

Unlikely events matter. Massive earthquakes, giant hurricanes, global financial crises, and pandemics are just a few examples of events that are rare but have catastrophic consequences. There are also many other situations in which the occurrence of a rare event is less dramatic but important nonetheless: for instance, typical electronic components are required to be extremely reliable, with a very low probability of failure, as are many other engineering devices used in the automobile, aerospace, and medical industries. In all of these examples, it is desirable to accurately estimate the probability and rate of occurrence of rare events. Large deviation theory (LDT) is the right framework to address these questions in many situations: LDT gives not only the desired probability of the event, but also its most likely pathway (MLP) of occurrence, which is often predictable. In this talk I will describe numerical tools that can be built upon LDT, permit to compute the MLP and can be integrated in importance sampling Monte Carlo sampling techniques and/or data assimilation strategies to dramatically improve their efficiency. I will also illustrate these tools on examples arising in various applications, including molecular dynamics, material sciences, and geophysical flows.

Martin Evans *Speed selection in coupled Fisher waves*

The Fisher equation describes the spread of a population or the spread of an advantageous gene through a population. It is well known as a simple nonlinear equation which exhibits travelling wave solutions. A selection mechanism for the speed of these waves has been established some time ago. We consider two coupled Fisher equations representing two populations e.g. sub-populations of bacteria which are susceptible or resistant to antibiotic. We show that a subtle coupling between two population waves gives rise to a novel velocity selection mechanism.

Tobias Galla *Stochastic processes with distributed delays: chemical Langevin equation and linear-noise approximation*

In this talk I will discuss a systematic approach to the linear-noise approximation for stochastic reaction systems with distributed delays. Unlike most existing work this formalism does not rely on a master equation, instead it is based upon a dynamical generating functional describing the probability measure over all possible paths of the dynamics. We derive general expressions for the chemical Langevin equation for a broad class of non-Markovian systems with distributed delay. Exemplars of a model of gene regulation with delayed auto-inhibition and a model of epidemic spread with delayed recovery provide evidence of the applicability of our results.

References:
T. Brett, T. Galla, Phys. Rev. Lett. 110, 250601 (2013)
T. Galla, Phys. Rev. E 80, 021909 (2009)

A.N. Gorban *Hierarchy of Dominant Paths in Multiscale Networks*

Joint work with A. Zinovyev and O. Radulescu

We consider multiscale networks of transport processes and approximate their dynamics by the systems of simple dominant networks. The dominant systems can be used for direct computation of steady states and relaxation dynamics, especially when kinetic information is incomplete. It could serve as a robust first approximation in perturbation theory or for preconditioning. Many of the parameters of the initial model are no longer present in the dominant system: these parameters are non-critical. Parameters of dominant systems indicate putative targets to change the behavior of the large network and answer an important question: given a network model, which are its critical parameters? The dominant system is, by definition, the system that gives us the main asymptotic terms of the stationary state and relaxation in the limit for well separated rate constants. The theory of dominant systems for networks with first-order kinetics and Markov chains is well developed [1, 2]. We found the explicit asymptotics of eigenvectors and eigenvalues. All algorithms are represented topologically by transformation of the graph of networks (labeled by the transport coefficients. In the simplest cases, the dominant system can be represented as dominant path in the network. In the general case, the hierarchy of dominant paths in the hierarchy of lumped networks is needed. Accuracy of estimates is proven. Performance of the algorithms is demonstrated on simple benchmarks and on multiscale biochemical networks. These methods are applied, in particular, to the analysis of microRNA-mediated mechanisms of translation repression [3].
For nonlinear networks, we present a new heuristic algorithm for calculation of hierarchy of dominant paths. Our approach is based on the asymptotic analysis of fluxes on the Volpert graph [4].
The results of the analysis of the dominant systems often support the observation by Kruskal [5]: “And the answer quite generally has the form of a new system (well posed problem) for the solution to satisfy, although this is sometimes obscured because the new system is so easily solved that one is led directly to the solution without noticing the intermediate step.”

References:
[1] A.N. Gorban, O. Radulescu, A.Y. Zinovyev, Asymptotology of chemical reaction networks, Chemical Engineering Science 65 (2010), 2310–2324,
[2] A.N. Gorban and O. Radulescu, Dynamic and Static Limitation in Multiscale Reaction Networks, Revisited, Advances in Chemical Engineering 34 (2008), 103–173.
[3] N. Morozova, A. Zinovyev, N. Nonne, L.-L. Pritchard, A.N. Gorban, and Annick Harel-Bellan, Kinetic signatures of microRNA modes of action, RNA 18 (9) (2012), 1635–1655.
[4] A.I. Vol’pert, Differential equations on graphs, Mathematics of the USSR–Sbornik 17 (4) (1972), 571–582.
[5] M.D. Kruskal, Asymptotology, In: Mathematical Models in Physical Sciences, ed. by S. Dobrot, Prentice-Hall, New Jersey, Englewood Cliffs, pp. 17–48, 1963.

Malte Henkel *Physical ageing in systems without detailed balance*

Physical aging was introduced to physics in Struik's ground-breaking experiments on reproducible and universal properties in glasses. Since then, spontaneously occurring relaxations in numerous many-body systems far from equilibrium have been systematically investigated. It has turned out that physical aging can be characterised by the simultaneous properties of (i) slow relaxation, (ii) breaking of time-translation-invariance and (iii) dynamical scaling. This motivates to try to draw analogies with conformal invariance at equilibrium critical points and to investigate on the possibility of local extensions of dynamical scaling, with a generic dynamical exponent z. A survey on systems undergoing physical aging and their recognised local dynamical symmetries will be given, but we shall concentrate on non-glassy systems. We shall see that so-called `logarithmic' extensions of standard dynamical scaling are often required. Kinetic Glauber-Ising models, the one-dimensional Kardar-Parisi-Zhang equation and one-dimensional directed percolation will serve as paradigmatic examples. New results on semi-infinite substrates will be presented.

Satya Majumdar *Number of Distinct and Common sites visited by N random walkers*

I'll discuss first the average number of distinct and common sites visited by N independent random walkers in d dimensions. The asymptotic temporal growth of the mean number of common sites displays an interesting phase diagram in the (N-d) plane: three phases separated by two critical lines at (i) d=2 and (ii) $d=d_c(N)= 2N/(N-1)$. In one dimension, we can compute the full distribution of the number of distinct and common sites visited by N walkers by mapping this problem to an extreme statistics problem. The universality of the scaling functions and application to ecology would be discussed.

Alan McKane *Are there species smaller than 1 mm?*

Intrinsic noise in systems with a large number of individuals often gives rise to complex structures on the macroscale. We review the mathematical formalism underlying the modelling of these effects, beginning with a description of the system in terms of its basic constituents. We illustrate the use of the formalism in a number of areas, especially in cases where the multiplicative nature of the noise plays an important role. We end by showing that stochastic effects can lead to the spontaneous formation of species in models of competing organisms. We argue that the result implies that ecospecies formation will be much more likely for megafauna than for meio or microfauna.

Vassili Kolokoltsov *Bose-Einstein condensation in number theory and economics*

We shall discuss some relations between number theory, physics and economics related to the notion of the Bose-Einstein condensation.

Tobias Kuna
Typical behaviour of extremes of chaotic dynamical systems for general observables

In this talk we discuss the distribution of extreme events for a chaotic dynamical system for a general class of observables. More precisely, we link directly the distribution of events over threshold to the scaling behaviour of the invariant distribution on the surface of the attractor.

Our considerations focus on observables for which the maximal value is not in the interior of the attractor. It is shown how this can provide us with information about the local stable and unstable dimensions. Using Ruelle's response theory, we discuss the sensitivity of the parameters of the distribution under perturbations. This is a joint work with Vlaerio Lucarini, Davide Faranda and Jeroen Wouters.

Mauro Mobilia *Coexistence and metastability in evolutionary games*

Evolutionary game theory (EGT), where the success of one species depends on what the others are doing, provides a promising framework to investigate the origin of cooperative behaviour and the mechanisms allowing the maintenance of species diversity. The classic approach to EGT is in terms of mean field replicator equations. It is however well established that evolutionary dynamics is generally affected by demographic noise and by the population's spatial arrangement. Evolutionary games in finite populations are often characterised by their fixation properties, which refers to the possibility that a few "mutants" take over the entire population. The fixation probability and mean fixation times are often computed within a diffusion approximation (Fokker-Planck equation), which is legitimate when the dynamics is not governed by large fluctuations but questionable otherwise.

After a cursory introduction to EGT, I will first focus on finite and well-mixed (spatially-homogeneous) populations and present a WKB (Wentzel-Kramers-Brillouin) based theory to describe the non-diffusive effects of the underlying dynamics. The WKB approach is particularly suited to fixation phenomena induced by large fluctuations and is here illustrated for a class of games characterised by the (metastable) coexistence of species. By comparing the predictions of the WKB and diffusion theories, the former is found to be superior when the selection intensity is finite whereas the latter is accurate in the weak selection limit. In the final part of this talk, I will discuss the influence of heterogeneous graphs on the metastability and fixation properties of a set of evolutionary processes. I shall particularly focus on the dynamics of snowdrift games (with metastable coexistence state) on scale-free networks. In the limit of weak selection, using an effective diffusion theory and by exploiting a time-scale separation, it will be shown that the scale-free structure affects the system's metastable state and leads to anomalous fixation properties. In particular, the probability and mean time of fixation are characterised by stretched exponentials with exponents depending non-trivially on the network's degree distribution.
References:
- EPL (Europhysics Letters) 91, 10002 (2010)
- J. Stat. Mech. P09009:1-24 (2010)
- Phys. Rev. Lett. 109, 188701 (2012)

David Mukamel *Long-Range correlations in driven, non-equilibrium systems*

Systems driven out of thermal equilibrium often reach a steady state which under generic conditions exhibits long-range correlations. Two systems which exhibit drive induced long-range effects are presented. It is shown that in two and higher dimensions the presence of a localized drive in an otherwise diffusive system results in steady-state density and current profiles which decay algebraically to their global average value, away from the drive. The same is true for the density-density correlation function. In the second class of systems, the effect of a localized drive on the steady state of an interface separating two phases in coexistence is considered. It is demonstrated that in d=2 dimensions drive along the interface induces spontaneous symmetry breaking of the interface, whereby its fluctuations into the two coexisting phases become non-symmetric.

Marco Sarich *The rebinding effect and reduced models for ligand binding processes*

The rebinding effect is a phenomenon which occurs when observing a ligand-receptor binding process. It refers to the fact that a ligand that has just dissociated from a receptor rebinds with a much higher probability compared to the binding probability of a ligand being far away from the receptor. We will discuss how this memory effect can spoil estimates for reaction rates or probabilities of the binding process. Further, we will show how to derive accurate reaction probabilities and reduced models for the binding process based on a weak definition of bound and unbound macro states.

Andreas Schadschneider *Exclusive queueing process: The dynamics of waiting in line and other jamming phenomena in pedestrian dynamics*

The dynamics of pedestrian crowds has been studied intensively in recent years, both theoretically and empirically. However, in many situations pedestrians movement can be rather static, e.g. due to jamming near bottlenecks or queueing at ticket counters or the supermarket checkout.

Classically such queues are often described by a M/M/1 queue. However, this stochastic process neglects the internal structure (density profile) of the queue by focussing on the queue length as the only dynamical variable. This is different in the exclusive queueing process (EQP) which generalizes the M/M/1 queue by considering the queue on a microscopic level. It is equivalent to a totally asymmetric exclusion process (TASEP) of varying length for which many exact results can be obtained. The EQP has a surprisingly rich phase diagram with respect to the arrival probability α and the service probability β. The behavior on the phase transition line is much more complex than that of the TASEP. It is nonuniversal and depends strongly on the update procedure used.

Gunter Schuetz *Diffusion in a slowly varying potential*

The equation which describes a particle diffusing in an attractive logarithmic potential arises in diverse physical problems such as momentum diffusion of atoms in optical traps, condensation processes, and denaturation of DNA molecules. A detailed study of the approach of such systems to equilibrium via a scaling analysis is carried out, revealing three surprising features: (i) the solution is given by two distinct scaling forms, (ii) the scaling exponents and scaling functions corresponding to both regimes are selected by the initial condition; and (iii) this dependence on the initial condition manifests a ``phase transition'' from a regime in which the scaling solution depends on the initial condition to a regime in which it is independent of it. We also consider the presence of Sinai-disorder in a slowly decaying repulsive power-law potential where an intriguing weak localization occurs.

Didier Sornette
Black Swans, Dragons and Predictions: Diagnostics and Forecasts for the World Financial Crisis (Colloquium)

Reverse-engineering of financial markets by agent-based models: regime shifts and breakdown of market efficiency

Julien Tailleur *Revisiting the flocking transition using Active Spins*

I will present an active Ising model in which spins both diffuse and align on lattice in one and two dimensions. The diffusion is biased so that plus or minus spins hop preferably to the left or to the right, which generates a flocking transition at low temperature/high density. Using a coarse-grained description of the model, I will show this transition to be a first-order liquid-gas transition in the temperature-density ensemble, with a critical density sent to infinity. In this first-order phase transition, the magnetization is proportional to the liquid fraction and thus varies continuously throughout the phase diagram. While this scenario is verified in microscopic simulations in 2d, the fluctuations alter the transition in 1d, preventing for instance any spontaneous symmetry breaking.

Victor Yakovenko
Statistical Mechanics of Money, Income, Debt, and Energy Consumption

By analogy with the probability distribution of energy in physics, entropy maximization results in the exponential Boltzmann-Gibbs probability distribution of money among the agents in a closed economic system. Analysis of empirical data shows that income distributions in USA, EU, and other countries have a well-defined two-class structure. The majority of the population (about 97%) belongs to the lower class characterized by the exponential ("thermal") distribution. The upper class (about 3% of the population) is characterized by the Pareto power-law ("superthermal") distribution, and its share of the total income expands and contracts dramatically during bubbles and busts in financial markets. Globally, inequality in energy consumption per capita around the world has decreased in the last 30 years and now approaches to the exponential probability distribution, in agreement with the maximal entropy principle. All papers are available at
http://physics.umd.edu/~yakovenk/econophysics/