Abstracts

Nigel Wilding (Bath) Three-body interactions in complex fluids

ABSTRACT: A simulation technique is described for quantifying the contribution of three-body interactions to the thermodynamical properties of coarse-grained representations of complex fluids. The method is based on comparing the third virial coefficient for a complex fluid with that of an approximate coarse-grained model described by a pair potential. To obtain the third virial we introduce a new technique which expresses its value in terms of the measured volume-dependent asymptote of a certain structural function. This same function also provides an appropriate coarse-grained pair potential representation of the fluid. The strategy is applicable to both Molecular Dynamics and Monte Carlo simulation. Its utility is illustrated via measurements of three-body effects in models of star polymer and highly size-asymmetrical colloid-polymer mixtures.

Douglas Ashton (Bath) Low density liquids with lock & key binding

ABSTRACT: When mixed with a small particle depletant spherical colloids with an indentation can form strong bonds whereby the indented side of one particle (the lock) fits neatly on the convex side of another (the key). For strong enough interactions the particles will form chains and branches depending on the precise geometry. We have mapped simulations of the full mixture to a greatly simplified model allowing us to study the phase behaviour of large systems. As the ratio between directional and non-directional binding increases the liquid phases become very stringy with the critical points moving to very low density. The resulting liquids have a rich, open structure with interesting percolation properties.

Juanpe Garrahan (Nottingham) Glass versus overlap transitions

ABSTRACT: A key open question in the glass transition field is whether a finite temperature thermodynamic transition to the glass state exists or not. Recent simulations of coupled replicas in atomistic models have found signatures of a static transition as a function of replica coupling. This can be viewed as evidence of an associated thermodynamic glass transition in the uncoupled system, as predicted by mean-field theory. I will describe a different scenario which emerges from the study of a class of idealised lattice models. I will consider the connection between thermodynamic overlap transitions and the active-inactive trajectory transitions revealed by the s-ensemble method, and will discuss what these results tell us about the glass transition problem more generally.

Mike Evans (Leeds) How physical is a constrained-path ensemble? On defining and analysing non-equilibrium states

ABSTRACT: A recent project [1] investigated the correspondence between a non-equilibrium ensemble defined via a distribution of phase-space paths, and a system driven into a steady-state by non-equilibrium boundary conditions. In doing so, we established effective protocols for analysing transition rates in non-equilibrium quasi-steady states. As well as presenting the results of that investigation, I will use the project as a case study, to refine some questions such as what is meant by distance from equilibrium, and how to measure non-equilibrium statistical mechanics.


Mike Moore (Manchester) Glasses and Jamming: lessons from hard disks in a narrow channel

ABSTRACT: The thermodynamic properties of disks moving in a channel sufficiently narrow that they can only collide with their nearest neighbors can be solved exactly by determining the eigenvalues and eigenvectors of an integral equation. Using it we have determined the correlation length $\xi$ of this system. We have developed an approximate solution which becomes exact in the high density limit. It describes the system in terms of defects in the zigzag arrangement of disks found in the high-density limit. The correlation length is then effectively the spacing between the defects. The time scales for defect creation and annihilation are determined with the help of transition state theory as is the diffusion coefficient of the defects and they are in good agreement with molecular dynamics simulations. On compressing the system with the Lubachevsky-Stillinger procedure jammed states are obtained whose $\phi_J$ are a function of the compression rate $\gamma$. We can quantitatively explain this
dependence by using the Kibble-Zurek hypothesis. We have also determined the point-to-set length scale for this system and it is much smaller than $\xi$ with a completely different dependence on the packing fraction.

The case of wider channels in which the disks can interact with their next-nearest neighbours can also be studied by similar methods. It has features not seen in the nearest-neighbour case, but which seem to be present in three dimensional jammed states of hard spheres.

David Saad (Aston) Self-sustained Clusters in Spin Models and their Link to Ergodicity Breaking

ABSTRACT: We study the entropy of self-sustained spin clusters in disordered systems, where in-cluster local fields are dominated by cluster spins and are therefore difficult to destabilise. Self-sustained spin clusters are shown to be analytically linked to ergodicity breaking in fully connected Ising and Sherrington-Kirkpatrick (SK) models, relating the less understood spin space characteristics to the well understood macroscopic state space properties. This correspondence is established through the absence of clusters in the paramagnetic phase, the presence of one dominant cluster in the Ising ferromagnet, and the formation of a non-trivial profile of self-sustained clusters in the SK spin glass. Yet unobserved phenomena are also revealed such as a first order phase transition in cluster sizes in the SK ferromagnet. The analysis was carried out under the replica symmetric and one-step replica symmetry breaking ansätze and could be adapted to investigate other spin models.


Richard Morris (Warwick), Tim Rogers (Bath) Growth driven dynamics in mean-field models of interacting spins

ABSTRACT: In this talk I will present results on two canonical models of statistical mechanics (the fully-connected voter and Glauber-Ising models), modified to incorporate the effects of growth. The interplay between relaxation and growth induces new behaviour in these systems: absorbing states of the voter model become metastable under constant growth, and vice-versa for the Glauber-Ising case. For accelerating growth, the dynamics of the voter model slow asymptotically to a halt, the distribution of states converging to that of a non-growing system, frozen at a known finite time.

Chris Fullerton (Bath) Randomly pinning particles in supercooled liquids and stable glasses: dynamic correlations and amorphous order

ABSTRACT: We investigate the response to randomly pinning particles in equilibrium configurations of a supercooled liquid and configurations from stable glassy states associated with large deviations in the dynamical activity. The distribution of the overlap between configurations sharing pinned particles reveals the presence of amorphous order in the glassy states. This helps to explain their stability. We also investigate the behaviour of four-point correlations as the number of pinned particles is increased.

Ian Thompson (Bath) Dynamic phase transitions in 1D hard systems

ABSTRACT: We analyse dense systems of hard particles in one dimension, by biasing towards trajectories with low (or high) dynamical activity. We observe several kinds of dynamical phase transition, some of which are similar to those found in glassy systems. On biasing to lower than average activity, we find phase separation in the constant density system, while the constant pressure system undergoes a jamming transition. For higher than average activity, the systems exhibit hyperuniformity. This explores the relationship between dynamical phases and structure as well as between jamming and glassy behaviour.

Robert Turner (Nottingham) An analogous Jarzynski relation in dynamical ensembles

ABSTRACT: Recently, there has been growing interest in extending the statistical mechanics approach from static configurations to trajectories. In this approach, the generating function of a dynamical process is basically interpreted as a partition sum. Here we go a step further and make a first connection to fluctuation theorems. We show that an effective dynamics in the space of trajectories, using a path sampling scheme, gives rise to the celebrated Jarzynski relation connecting a meta-work with the change of the generating function. We demonstrate the potential applicability of this result to computer simulations for two open quantum systems, a two-level system and the micromaser. We finally discuss the behavior of the Jarzynski relation across a first-order phase transition.
Silvia Bartolucci, Alessia Annibale (KCL) Dynamics of associative networks with diluted patterns

Associative networks with diluted patterns have been recently introduced as a generalisation of the standard Hopfield model. In addition to their relevance in artificial intelligence, these models are increasingly important in immunology, where stored patterns represent strategies to fight pathogens and nodes represent lymphocyte clones. In this work we solve the dynamics of pattern diluted associative networks, evolving via sequential Glauber update. We derive dynamical equations for the order parameters, that quantify the simultaneous pattern recall of the system, and analyse the nature and stability of the stationary solutions by means of linear stability analysis as well as Monte Carlo simulations. We investigate the parallel retrieval capabilities of the system in different regions of the phase space, in particular in the low and medium storage regimes and for finite and extreme pattern dilution. Results show that in the absence of patterns cross-talk, all patterns are recalled symmetrically for any temperature below criticality, while in the presence of pattern cross-talk, symmetric retrieval becomes unstable as temperature is lowered and a hierarchical retrieval takes over. The parallel retrieval capabilities of the network are seen to degrade gracefully in the regime of strong interference, but they are not destroyed.

James Barrett (KCL) Multiple output Gaussian process regression for analysing survival analysis with competing risks

ABSTRACT: The competing risks problem can be regarded as a regression problem with multiple outputs (the event times) that may be statistically dependent. Multiple output Gaussian process (GP) regression is a flexible probabilistic non-parametric method of inferring non-linear relationships between covariates and multiple outputs. It is shown how GP regression can be applied to survival analysis with competing risks. The model is capable of detecting and exploiting dependencies between risks. This approach does not require any explicit assumption on what form the hazard rates take. Estimates of times for events that were censored can be generated along with survival curves and hazard rates.

Richard Blythe (Edinburgh) Parasites on parasites: coupled fluctuations in stacked contact processes

ABSTRACT: We present a model for host-parasite dynamics which incorporates both vertical and horizontal transmission as well as spatial structure. Our model consists of stacked contact processes (CP), where the dynamics of the host is a simple CP on a lattice while the dynamics of the parasite is a secondary CP which sits on top of the host-occupied sites. In the simplest case, where infection does not incur any cost, we uncover a novel effect: a non-monotonic dependence of parasite prevalence on host turnover. Inspired by natural examples of hyperparasitism, we extend our model to multiple levels of parasites and identify a transition between the maintenance of a finite and infinite number of levels, which we conjecture is connected to a roughening transition in models of surface-growth.

Justin Whitehouse (Edinburgh) Don’t Forget Your Tail! A Moving Condensate Maintained by its Tail

ABSTRACT: Condensate phases, where some quantity becomes localised, are found in fundamental models of a wide variety of processes, such as in traffic flow, wealth redistribution, etc. Within the ‘standard’ formulation of the Zero-Range Process (ZRP), where only one unit of mass ‘hops’ at a time, a condensation transition is observed with the appropriate choice of hop rate. However, condensates formed in this model are static, whereas many real-world systems exhibit a moving condensate phase, such as a traffic jam. To learn more about moving condensate phases we study a model based on the ZRP where all but one of the particles on a site hop at once. We find that under these dynamics a moving strong condensate is formed at all densities ρ when a hopping parameter b is increased beyond a critical value b_c. We show using analytical and numerical approaches that the model exhibits a stable moving condensate localised over a few lattice sites.

Tanguy Laffargue (Paris, Diderot) Chaoticity fluctuations in diffusive systems

ABSTRACT: Many physical phenomena can be described as a phase transition between very different regimes. For instance, the onset of turbulence goes hand in hand with the emergence of chaotic trajectories in an otherwise regular flow. Perhaps less obvious is that the glass transition can be interpreted in terms of a transition from diffusive dynamics to an arrested, frozen-in, and ergodicity-breaking regime. In addition, typical configurations of a system can result from the superposition of structures of different dynamical properties.

A natural observable to quantify the chaoticity of a trajectory is the Lyapunov spectrum, and it then appears as a good candidate to sort trajectories, hence discriminating between different dynamical regimes. By analogy with equilibrium thermodynamics, where the temperature allows us to select
the typical energy of configurations, a formalism has been developed to isolate trajectories of atypical
chaoticity. Instead of being based on configurations, this formalism lives in trajectory space and acts
much as a prism does with natural light: it decomposes the fundamental units of the dynamics.

While the ultimate and ambitious goal of this approach is to study the glass transition and identify the
much sought-after soft modes, for now, we are making the first few steps in this direction by considering
simplified models of colloidal systems.

Yuzuru Sato (Imperial/Hokudai) *Random dynamical systems approaches to noise-induced phenomena*
abstract: Noise-induced phenomena arise out of interaction between deterministic dynamics and
stochastic noise. Stochastic resonance, noise-induced synchronization, and noise-induced chaos are
typical examples in statistical and nonlinear physics. In this presentation, I discuss recently discovered
noise-induced phenomena from the random dynamical systems point of view. Applications to time-
series analysis of dynamical systems with a large degrees of freedom, based on experimental data of
rotating fluid, is also exhibited.

Rob Jack (Bath) *Information-theoretic measurements of coupling between structure and dynamics in glass-

ABSTRACT: Glass-forming liquids are dynamically heterogeneous: for a given initial condition, some
particles tend to be more mobile than others, on the time scales relevant for structural relaxation. We
analyse the extent to which particles’ motion can be predicted, based on the local structure of the
liquid. In particular, we measure the mutual information between a particle’s initial environment and
its ensuing motion, in order to test which aspects of the structure have the most predictive power for
dynamics. We discuss the consequences of these results for theories of the glass transition.

Tomaso Aste (UCL), Tiziana Di Matteo, Raffaello Morales, Nicolo Musmeci, (KCL) *Dependency
structure and scaling properties of financial time series are related*
ABSTRACT: Complexity of financial time series is associate with two main elements: the first is
multifractality [1], which is related with the behavior of each single variable and the way it scales in time;
the second is the structure of dependency between time series, associated with the collective behavior of
the whole set of variables [2,3]. So far, these two manifestations of complexity have been investigated
separately. In this talk I will point out that -in fact- they are related [4]. I will first introduce a
graph-theoretic approach to extract the hierarchical structure of inter-dependency between financial
variables in an unsupervised and deterministic manner, without the use of any prior information [2].
I will then discuss the existence of a deep interplay between cross-correlations hierarchical properties
and multifractality [4]. Showing in particular that the degree of multifractality displayed by different
stocks is positively correlated to their depth in the hierarchy of cross-correlations.


Pierpaolo Vivo (Orsay) *Phase transitions in the condition number distribution of Gaussian random ma-
trices*
ABSTRACT: We study the statistics of the condition number $k = \lambda_{max}/\lambda_{min}$ (the ratio between
largest and smallest squared singular values) of $N \times M$ Gaussian random matrices. Using a Coulomb
fluid technique, we derive analytically and for large $N$ the cumulative $P[k < x]$ and tail-cumulative
$P[k > x]$ distributions of $k$. We find that these distributions decay as $P[k < x]$ $\approx \exp(-\beta N^2 \Phi_-(x))$
and $P[k > x] \approx \exp(-\beta N \Phi_+(x))$, where $\beta$ is the Dyson index of the ensemble. The left and right
rate functions $\Phi_{\pm}(x)$ are independent of $\beta$ and calculated exactly for any choice of the rectangularity
parameter $\alpha = M/N - 1 > 0$. Interestingly, they show a weak non-analytic behavior at their minimum
$< k >$ (corresponding to the average condition number), a direct consequence of a phase transition in
the associated Coulomb fluid problem. Matching the behavior of the rate functions around $< k >$, we
determine exactly the scale of typical fluctuations $O(N^{-2/3})$ and the tails of the limiting distribution
of $k$. The analytical results are in excellent agreement with numerical simulations, obtained with a
sophisticated “reweighing” (adaptive) technique allowing to sample extremely rare occurrences.
Reimer Kühn, Peter Sollich (KCL) *Spectra of sample auto-covariance matrices*

ABSTRACT: We compute spectral densities of large sample auto-covariance matrices of stationary stochastic processes at fixed ratio $\alpha = N/M$ of matrix dimension $N$ and sample size $M$. We find a remarkable scaling relation which expresses the spectral density $\rho_\alpha(\lambda)$ of sample auto-covariance matrices for processes with correlations as a continuous superposition of copies of the spectral density $\rho^{(0)}_\alpha(\lambda)$ for a sequence of uncorrelated random variables at the same value of $\alpha$, rescaled in terms of the Fourier transform $\hat{C}(q)$ of the true auto-covariance function. We also obtain a closed-form approximation for the scaling function $\rho^{(0)}_\alpha(\lambda)$. Our results are in excellent agreement with numerical simulations using auto-regressive processes, and processes exhibiting a power-law decay of correlations.


Katy Rubin, Peter Sollich (KCL) *Boundary structure of gene regulation response in protein interaction subnetworks*

ABSTRACT: In large protein interaction networks or other networks in systems biology, it is often of interest to focus on the dynamics of a subnetwork embedded in a larger bulk network – e.g. because the bulk network may be incompletely known, because only a small number of molecular species can be tracked experimentally, or to make it easier to understand the dynamics qualitatively. We review briefly a description of such subnetwork dynamics derived using Zwanzig-Mori projection methods, which involves memory terms governing the evolution of species on the boundary of the subnetwork. We then apply this to the analysis of the effects of perturbations in the bulk network, e.g. from gene regulation processes. We show that the resulting behaviour can again be decomposed according to a boundary structure, so that the total response is split into the effect of the bulk perturbation on the subnetwork boundary and the "propagation" of the perturbation from there to the rest of the subnetwork.

Juan Pablo Neirotti (Aston) *Computational properties of Ultrametric Committee Machines*

ABSTRACT: The problems of learning by examples and storage capacity in ultrametric committee machines (UCMs) are studied within the framework of statistical mechanics. Using the replica formalism we calculate the average generalization error in UCMs with $L$ hidden layers and for a large enough number of units $K$. In most of the regimes studied we find that the generalization error, as a function of the number of examples presented, develops a discontinuous drop at a critical value of the load parameter. We also find that when $L<1$ a number of teacher networks with the same number of hidden layers and different overlaps induce learning processes with the same critical points.

We also found that, in the first replica-symmetry broken approach and by increasing the number of hidden layers, the asymptotic behaviour of the storage capacity approaches $O(K \log(K))$.

Tomaso Aste (UCL), Tiziana Di Matteo, Raffaello Morales, Nicolo Musmeci, (KCL) *Dynamical analysis of clustering on financial market data*

ABSTRACT: In this talk I will show the application of the DBHT method [1,2] to a set of 342 US stocks daily prices during the time period between 1997 and 2012. The DBHT method is a novel approach to extract cluster structure and to detect hierarchical organization in complex data-sets, it is based on the study of the properties of Planar Maximally Filtered Graphs (PMFG) [3,4], it is deterministic, requires no a-priori parameters and it does not need any expert supervision.

In the case of financial data, the method yields a clustering set of stocks and a hierarchical structure of correlations. I will discuss the dynamical evolution of these clusters and structures and show results about their persistence over time, together with analyses about their varying similarity with the ICB Industrial Sectors classification. These measures point out peculiar behaviours in coincidence with the 2007-08 financial crisis [5].

Aleksandra Aloric, Peter Sollich (KCL) *Spontaneous Segregation of Agents Across Double Auction Markets*

ABSTRACT: In this research we investigate the possibility of spontaneous segregation of traders into groups when faced with having to choose among several markets. In this talk I will outline the motivation, and introduce the problem. I will present the simplified model we use and results obtained during previous period, where even in the simplest case of two markets and Zero Intelligence traders, we are able to observe segregation effects below a critical value $T_c$ of the temperature $T$; the latter regulates how strongly the traders bias their decisions towards options with large accumulated scores. It is notable that segregation occurs even though the traders are statistically homogeneous. Additionally, I will present an analytical description of the system in the large trader population limit. Predictions from the resulting theory are in good qualitative agreement with simulation results, even though the latter are obtained for relatively small populations of traders.

Pierre Paga, Reimer Kühn (KCL) *Contagion in an interacting economy*

ABSTRACT: We investigate credit contagion in complex networks of economic dependencies. Expanding on former results, we show that the model is exactly solvable in the thermodynamic limit, $N \to \infty$, and that the exact solution is described by a message passing approach originally proposed by Karrer and Newman. We compare our solution with simulation results for scale-free graphs.