CENTRE DE RECERCA MATEMÀTICA

Joint CRM - Imperial College School and Workshop in Complex Systems

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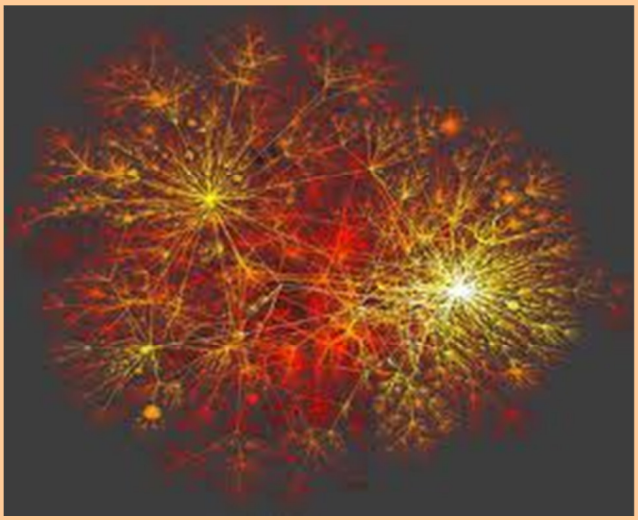

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Percolation in Complex Networks

Kim Christensen, Imperial College London

Critical Phenomena and Percolation Theory

Henrik J. Jensen, Imperial College London

Dynamics of Complex Systems (intermittency, stability, etc)

Gunnar Pruessner, Imperial College London

Non-Equilibrium Phase Transitions, Field Theory and Self-Organised Criticality

M. Ángeles Serrano, Universitat de Barcelona

Complex Networks and Hidden Metric Spaces: Internet, Metabolic Networks

Antonio Turiel, CSIC

Multifractal Formalism: from models for turbulent flows to applications in ocean remote sensing

Public Lecture

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POSTERS

Ana Elisa Bergues Pupo[1,2] **Alessandro Fiasconaro**[1,3]**, Fernando Falo**[1,4]

Mesoscopic model for the overstretching transition of DNA.

Abstract: A mesoscopic model for the overstretching transition of DNA is presented. Model is based in a discrete version of a worm-like chain model with elastic modifications. The model presented is able to describe the full stretching features of a DNA chain under dynamical conditions. A very good agreement between simulation and experiment is obtained. [1]

The first results of an extended model that take into account force induced melting during overstretching transition based on the Peyrard-Bishop-Daxois model will be also presented. This approach could clarify and possibly discriminate the occurrence of the two different DNA overstretched conditions: the ladder-like DNA (S-DNA) and molten DNA (M-DNA).

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Valentino Bianco and Giancarlo Franzese

Hydrophobic confinement: effect on a supercooled water monolayer.

Abstract: Water is extremely important for life and, at the same time, very anomalous with respect to simple substances. Different theories have been proposed in order to explain tho origin of such anomalies. A way to discriminate between these theories is to analyze, with experiments and simulations, the behavior of metastable supercooled water. In particular it has been suggested that water under confinement at low temperatures could be related to highly supercooled bulk water.

We contribute to the debate by analyzing the behavior of a water monolayer confined between hydrophobic walls. By cluster Monte Carlo simulations, based on a mathematical mapping in a percolating system, we are able to simulate extremely large systems for extremely long time scales, finding the anomalies and relating them to the low temperature phase diagram. We find a first order phase transition line separating two metastable liquids: the high-density liquid (HDL) at higher temperatures and pressures and the lowdensity liquid (LDL) at lower temperatures and pressures. Such line ends in a liquid-liquid critical point (LLCP). By finite size scaling of the appropriate order parameter, we find that the LLCP belongs to the universality class of the two-dimensional (2D) Ising model in the limit of infinite walls. However, for wall sizes up to fifty times larger than the monolayer thickness h, the LLCP is better described by the 3D Ising model universality class, something unexpected based on studies for simple liquids. We ascribe this result to the strong cooperativity and the low coordination number of the hydrogen bond network.

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Anna Deluca[1,2], Pere Puig[2] y Álvaro Corral[1]

Testing Universality and goodness-of-fit test of power-law distributions.

Abstract: Power-law distributions contain precious information about a large variety of physical processes. Although there are sound theoretical grounds for these distributions, the empirical evidence giving support to power laws has been traditionally weak. Recently, Clauset et al. have proposed a systematic method to find over which range (if any) a certain distribution behaves as a power law. However, their method fails to recognize true (simulated) power-law tails in some instances, rejecting the power–law hypothesis. Moreover, the method does not perform well when it is extended to power-law distributions with an upper truncation.

We present an alternative procedure, valid for truncated as well as for non-truncated powerlaw distributions, based in maximum likelihood estimation, the Kolmogorov-Smirnov goodness-of-fit test, and Monte Carlo simulations. We will test the performance of our method on several empirical data which were previously analyzed with less systematic approaches. The databases include the half-lives of the radionuclides, the seismic moment of earthquakes worldwide and in Southern California, a proxy for the energy dissipated by tropical cyclones, and the repetitions of words in texts (testing the validity of Zipf's law). We find the functioning of the method very satisfactory.

In addition, we will compare the estimated critical exponents in order to test the existence of a single universal exponent. We will do that by constructing confidence intervals on the exponent differences and by means of the Permutation test.

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Francesc Font-Clos[*1], **Francesco A. Massucci**[2], **Isaac Pérez Castillo**[3]

Modeling metabolic networks through a weighted belief-propagation algorithm.

Abstract: Many problems from a wide range of disciplines can be understood as counting the number of solutions to a set of either equalities or inequalities. In the following lines, we present a novel method to study some relevant properties of these systems using a probabilistic approach.

Focusing here on metabolic networks, we consider a system of $i = 1 \dots N$ coupled chemical reactions which produces and consumes $\mu = 1 \dots M$ metabolites and exchanges them with the environment. For each metabolite $\mu = 1 \dots M$, the associated dynamic mass balance equation reads

$$\frac{d}{dt}C^{\mu}(t) = \sum_{i=1}^{N}(a_i^{\mu} - b_i^{\mu})x_i(t) + (i^{\mu}(t) - o^{\mu}(t)) \tag{1}$$

where $C^{\mu}(t)$ is the concentration of metabolite μ at time t, $A = (a_i^{\mu})$ $(B = (b_i^{\mu}))$ are the output (input) stoichiometric matrices, $x_i(t)$ is the rate of reaction i and $i^{\mu}(t)$ $(o^{\mu}(t))$ is the input (output) exchange rate with the environment (associated to e.g. transport of metabolites).

Under the reasoning that the time-scales governing metabolic processes are much faster than those governing genetic regulation, one can assume steady metabolic concentrations, as well as steady reaction fluxes and exchange rates. Hence, denoting $\xi_i^{\mu} = a_i^{\mu} - b_i^{\mu}$ and $\gamma^{\mu} = o^{\mu} - i^{\mu}$, equation (1) becomes a set of equalities for the reaction rates, viz.

$$\sum_{i=1}^{N} \xi_i^{\mu} x_i = \gamma^{\mu}, \quad \forall \mu = 1 \dots M \tag{2}$$

From a mathematical viewpoint, the set of equations (2) together with a set of bounds $[x_i^{\min}, x_i^{\max}] \ni x_i$ defines a polytope in $\mathbb{R}^N$ of feasible solutions. The volume V of this polytope can be formally written as:
$V = \int_D d\boldsymbol{x} \prod_{i=1}^{M} \delta\left(\sum_{i=1}^{N} \xi_i^{\mu} x_i - \gamma^{\mu}\right)$ where $D = \times_{i=1\dots N}[x_i^{\min}, x_i^{\max}]$ is the integration domain. Unlike well-known techniques such as Flux Balance Analysis[1], where the whole volume is approximated by a single point, we aim here at dealing with the distribution of the volume V along each axes or, in other words, the marginal pdf $P_i(x_i)$:

$$P_i(x_i) = \frac{1}{V}\int_D d\boldsymbol{x}_{\setminus i} \prod_{i=1}^{M} \delta\left(\sum_{i=1}^{N} \xi_i^{\mu} x_i - \gamma^{\mu}\right) \tag{3}$$

where $\boldsymbol{x}_{\setminus i}$ denotes the vector $\boldsymbol{x}$ without component i. In practical situations, the stoichiometric matrix $\boldsymbol{\xi} = (\xi_i^{\mu})$ is generally diluted, meaning that its associated bipartite graph is tree-like. This allows us to use the cavity method[2] and derive

the following set of self-consistency equations:

$$m_\mu^{(i)}(x_i) = \int d\boldsymbol{x}_{\partial\mu\setminus i}\, \delta\left(\gamma^\mu - \sum_{j\in\partial\mu} \xi_j^\mu x_j\right) \prod_{j\in\partial\mu\setminus i} P_j^{(\mu)}(x_j) \tag{4}$$

$$P_i^{(\mu)}(x_i) = \frac{1}{Z_i^{(\mu)}} \prod_{\nu\in\partial i\setminus\mu} m_\nu^{(i)}(x_i) \tag{5}$$

where $Z_i^{(\mu)}$ are normalization constants, $\partial\mu$ stands for the neighborhood of node μ, and the set of functions $\{m_\mu^{(i)}(x_i), P_i^{(\mu)}(x_i)\}_{i\in\partial\mu}$ can be understood as messages between node i and node μ. The real marginals, that is, the pdf of our network's reaction fluxes, can be recovered from the messages through the relationship $P_i(x_i) = \frac{1}{Z_i}\prod_{\mu\in\partial i} m_\mu^{(i)}(x_i)$.

We propose to solve the self-consistency equations (4, 5) by means of a novel weighted population dynamics scheme. In a nutshell, population dynamics is a way of performing Monte Carlo integration when the integrand is unknown: each cavity density $P_i^{(\mu)}(x_i)$ is represented by a population of $\mathcal{N}_p$ pairs $\{(w_{i,\alpha}^{(\mu)}, x_{i,\alpha}^{(\mu)})\}_{\alpha=1}^{\mathcal{N}_p}$. Then, equation (4) translates into a dynamical process for the populations (see [3] for details). It can be shown that, starting with random initial conditions, this process converges to a stationary state, where the densities are recovered from the populations through

$$P_i^{(\mu)}(x_i) \approx \frac{1}{\Omega_i^{(\mu)}} \sum_{\alpha=1}^{\mathcal{N}_p} w_{i,\alpha}^{(\mu)} \delta\left(x_i - x_{i,\alpha}^{(\mu)}\right) \tag{6}$$

where $\Omega_i^{(\mu)} = \sum_{\alpha=1}^{\mathcal{N}_p} w_{i,\alpha}^{(\mu)}$ is the total weight. Once the cavity marginals are obtained, the same procedure is applied to obtain the final marginals.

The proposed method has been run[3] on theoretical random metabolic networks of small sizes, and its results compared with those obtained by crude Monte Carlo methods such as the Hit-and-Run algorithm [4].

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Wojciech Ganczarek

Single infection epidemics spreading model.

Abstract: Most of epidemics spreading models on graphs are based on an idea that during a particular time step each vertex is able to contaminate any number of its neighbors with a finite probability. This kind of assumption seems to allow us to tread the system being investigated by continous approximation, mainly: describing dynamics by differential equations. This, however, need not to be the case. We propose a model allowing only one infection per time step and analyze it in discrete manner. Theoretical and simulational results for epidemics treshold, stationary state and mixing time will be shown. And, although one contamination per time step may seem not that realistic, we will try to convince you that there actually exist corresponding systems in society.

Manuel Jurado

Negative-feedback self-regulation contributes to robust high-fidelity transmembrane signal transduction.

Abstract: Transmembrane cellular signaling pathways are responsible for linking external stimuli and internal cellular actions. How spatio-temporal mechanisms, and in particular discretization of the signaling process in locally confined structures, influence signal transduction is not fully understood. Recently, transient membrane nanoclusters concentrating signaling proteins have been proposed as a new fundamental mechanism to modulate and increase the efficiency and specificity of the MAPK cascade. We address this issue [1] by presenting a simple motif model for transmembrane cell signaling that considers minimal signaling events taking place in spatially distributed membrane domains regulated by a spatio-temporal dynamics. Based on this model, stochastic simulations have been performed using realistic kinetic reaction constants. We find that complex behaviors attributed to the particular architecture of signaling pathways (cascades of distributed activations and feedback loops) can be also achieved by regulating the spatio-temporal dynamics of nanoclusters encapsulating much simpler signaling motifs. More specifically, nanocluster ultrasensitivity is regulated by its lifetime, and this in turn, modulates the fidelity of global signal transduction. To explore how cells might have protected the fidelity of signal transduction, two scenarios have been compared: a situation where the nanocluster lifetime is externally regulated, and the case where it is self-regulated by their local activity. In the latter case, we report that self-regulation induces robust individual ultrasensitivity behavior and high fidelity global responses for a wide range of kinetic parameters.

The presented approach is generic and modular, making the results relevant for a variety of signaling processes subjected to a spatio-temporal dynamics, and can easily accommodate modifications and extensions to tailor it to different specific problems.

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Kolja Kleineberg

Instanton approach to the inverse cascade of two-dimensional turbulence.

Abstract: We investigate two-dimensional turbulence within the Instanton formalism which determines the most probable field in a stochastic classical field theory starting from the Martin-Siggia-Rose path integral. We perform an approximate analysis of these equations based on a variational ansatz using elliptical vortices. The result are evolution equations for the positions and the shapes of the vortices. We solve these ordinary differential equations numerically. The extremal action for the two-point statistics is determined by the merging of two elliptical vortices. We discuss the relationship of this dynamical system to the inverse cascade process of two-dimensional turbulence.

The poster follows roughly the content of our recent paper (`http://pre.aps.org/abstract/PRE/v87/i3/e033007`).

Universitat de Barcelona.

O. V. Maslennikov & V. I. Nekorkin

Spatio-temporal patterns in a large-scale discrete-time neuron network.

Abstract: We propose a model of the vertebrate olivo-cerebellar system in the form of a discrete-time dynamical system. The networked model qualitatively reproduces the most important structural features of the biological prototype and dynamical activity of its components. We show there are some collective behavior types in the model corresponding to those observed experimentally and hypothesized to be responsible for motor control. Namely, we find that the discrete-time units interacting with each other can generate spontaneous and induced by external stimulation spatio-temporal patterns. Their characteristic size and spatial order depend on the model parameters, relative coupling strength and signal propagation delays. We test our model by calculating some quantities introduced in the theory of Markov random fields and utilized by experimentalists in in vitro studies of neural tissues. We find that the results obtained are in good qualitative agreement with experimental measurements of the olivo-cerebellar system activity.

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Joan del Castillo and Isabel Serra

Statistical model for critical phenomenon.

Abstract: A new statistical approach for modelling extremes values is applied to model the power dissipation index of tropical cyclones. The new methodology includes a non-parametric tool: CV-plot and a new family to model extremes values: the full-truncated gamma (FTG). This signifi cantly improves the fit obtained with the classical methodology: ME-plot and Pareto distribution. Also, FTG is obtained in the framework of exponential dispersion models.

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