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Field theoretic description of charge-regulation interaction

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In order to find the exact form of the electrostatic interaction between two proteins with dissociable charge groups in aqueous solution, we have studied a model system composed of two macroscopic surfaces with charge dissociation sites immersed in a counterion-only ionic solution[1]. We introduced a surface free energy corresponding to a simple model of charge regulation. Charge regulation is an old concept refering to the case, where the effective charge on a macroion, e.g. protein surface, responds to the local solution conditions, such as local pH, local electrostatic potential, salt concentration, dielectric constant variation and the presence of other charged groups. While in nanoscale interactions one often assumes constancy of surface macroion charge [2], in fact the charge state of the dissociable groups on the macroion surface always depends strongly on the acid-base equilibrium that defines the fraction of acidic (basic) groups that are dissociated and requires to be consistently included in any theoretical formulation. Due to it, we derived a theory, starting from the field-theoretic representation of the grand canonical partition function. It is evaluated within the mean field approximation giving the Poisson-Boltzmann theory with the Ninham-Parsegian boundary condition [3]. Gaussian fluctuations around the mean-field are then analyzed in the lowest order correction that we calculate analytically and exactly, using the path integral representation for the partition function of a harmonic oscillator with time-dependent frequency. Our general result gives attractive, long-ranged, fluctuation interaction which depends on the pH of the solution. The obtained attraction can overcome mean filed repulsion when the surfaces reach their point of zero charge (PZC). Taking the proper limits, our result reduces to the zero-frequency van der Waals term, but also gives the correct Kirkwood-Shumaker result [4]-[5], which opens up the possibility to investigate the Kirkwood-Shumaker interaction in more general contexts where their original derivation fails.



Figure 1: Graphical representation of the model: two charged planar surfaces with charge dissociation sites distributed uniformly along the surfaces and with counterions between the surfaces. The counterions originate from the charge dissociation of the dissociable groups (AC) through the reaction AC \leftrightarrow A⁻ + C⁺.

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Spin-based description of water in models of biological macromolecules

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When describing the peculiarities of H-bond formation between water and biopolymer repeated units under the assumptions that: a) the interaction is short ranged; b) external conditions (P,T) are far from water critical points and are limited to physiological range, it is possible to offer a limited description of water in terms of Potts spins. Though limited, it allows to achieve a qualitatively correct description of reentrance in the phase diagrams of biopolymers (protein folding, helix-coil transition or DNA melting). Since it is very simple, it allows a direct summation over solvent degrees of freedom, resulting in a renormalization of spin-spin interaction energy (coupling), which becomes temperature-dependent as a result (see, e.g. [1]). Using the exact form of this transformation in simulations is very promising. On the example of a hard-sphere polymer model with square-well potential we obtain the results that are qualitatively similar with studies of a much more complex computational models reported from the Debenedetti group [2]. Our approach can reproduce the observed cold and heat denaturation (as in Fig 1), but at a much smaller computational cost.



Figure 1: Average energy vs temperature, with the recalculated effect of water. Initial curve for hard sphere pentamer chain is shown in black, values of polymer-solvent interaction energy are shown.

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A self-organized method for risk perception in epidemic spreading on multiplex networks

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In this paper we study the interplay between epidemic spreading and risk perception on multiplex networks. The basic idea is that the effective infection probability is affected by the perception of the risk of being infected, which we assume to be related to the number of infected neighbors, as introduced in Ref. [1]. We re-derive the previous results using a self-organized method, that automatically gives the percolation threshold in just one simulation. We then extend the model to multiplex networks considering that people get infected by contacts in real life but often gather information from virtual social networks, that may be quite different from the real ones. The similarity between the real and virtual networks determine the possibility of stopping the infection for a sufficiently high precaution level: if the networks are too different there is no level of precaution capable of stopping the epidemics.

We are interested in studying numerically the dependence of the epidemic threshold on the parameters of the model. The determination of a percolation threshold is not a easy task to be automatized. We extend a self-organized formulation of percolation phenomena [2] that allows to obtain this threshold in just one simulation (for a sufficiently large system).

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Correlation between economic inequality and mobility in kinetic models for social sciences

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Statistical evaluations of the economic mobility of a society are more difficult than measurements of the income distribution, because they require to follow the evolution of the individuals' income for at least one or two generations. Correspondingly, in micro-to-macro theoretical models of economic exchanges based on kinetic equations, the income distribution depends only on the asymptotic equilibrium solution of the equations, while mobility estimates also involve the detailed structure of the transition probabilities of the model, and are thus an important tool for assessing its validity. Since empirical data show a remarkably general negative correlation between economic inequality and mobility, whose explanation is still unclear, it is particularly interesting to study this correlation in analytical models.

In our papers [1, 2, 3, 4, 5], a class of models is formulated for the description of the micro-processes of money exchange, taxation and redistribution in a closed market society, which are expressed by systems of differential equations of the kinetic discretized-Boltzmann kind. While traditional treatments of these and related subjects in mainstream economics rely on the assumption of a representative rational agent, our approach fits in with a complex system perspective. Society is described as an ensemble of individuals divided into a finite number of income classes; the individuals exchange money through binary and ternary interactions, leaving the total wealth unchanged. The ternary interactions represent the taxation and redistribution process: they express the subtraction, in correspondence to each binary transfer, of an amount whose percentage (tax rate) depends on the income classes of the individuals involved in the interaction; and they define the redistribution (also weighted according to a means-tested welfare system) of this amount to all other individuals. The frequencies with which the interactions occur as well as other parameters can be tuned so as to provide a probabilistic representation as realistic as possible. For instance, we can fix the probability that in an encounter between two individuals the one who pays is the rich or the poor, we can postulate that the exchanged amount depends on the income classes according to a variable saving propensity, etc. We show the emergence from the interplay of the individual interactions of observable collective patterns like the income distribution curve. Indeed, all computational simulations suggest that after a sufficiently long time the solution of the equations reaches an equilibrium state corresponding to an income distribution, which depends on the total wealth and on the interaction parameters, but not on the initial distribution and which exhibits fat tails as do the real world ones.

We investigate the behavior of the Gini inequality index in dependence on several parameters: saving propensity, taxation rates gap, tax evasion rate, welfare means-testing etc. In particular, by analyzing the dependence of mobility from the same parameters, we can check its intrinsic correlation with inequality. Our findings confirm that the correlation is negative and highlight interesting relationships between the indicators of the phenomena under consideration.

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Detrending Moving Average Algorithm: a Non-Random Walk through ComplexSystems Science

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Time series are a tool to describe biological, social and economic systems in one dimension, such as stock market indexes and genomic sequences. Extended systems evolving over space, such as urban textures, World Wide Web and firms are described in terms of high-dimensional random structures. A short review of the Detrending Moving Average (DMA) algorithm is presented. The DMA has the ability to quantify temporal and spatial long-range dependence of fractal sets with arbitrary dimension. Time series, profiles and surfaces can be characterized by the fractal dimension D, a measure of roughness, and by the Hurst exponent H, a measure of long-memory dependence. The method, in addition to accomplish accurate and fast estimates of the fractal dimension D and Hurst exponent H, can provide interesting clues between fractal properties, self-organized criticality and entropy of long-range correlated sequences. Further readings á0and tips about the DMA algorithm at www.polito.it/noiselab

Zipf's law and a scaling law, in texts and in music

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Zipf's law is considered one of the key statistical regularities of human language. We show that, in general, Zipf's power law does not hold for the whole domain of word frequencies, but only for the upper tail, i.e., for the most common words. On the other hand, the distribution of word frequencies changes with the size of the text in such a way that it scales with the size of the text and the size of the vocabulary; this means that the shape of the distribution does not change with system size, only its scale changes, providing a recipe for the proper comparison of texts of different size [1], see figure. The distinction between the terms "power law" and "scaling law" is fundamental here. A second part of the talk will be devoted to the extension of Zipf's law to music, drawing parallelisms and differences with texts. The construction of music code-words from the chords defining the pitch in modern popular music reveals the validity of Zipf's law in this case. This law has kept stability for the last 50 years, although other characteristics of music have shown an evolution that seems to indicate a decrease of the complexity of music with time [2].

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Figure 1: Left: Probability mass function $D_L(n)$ versus word absolute frequency *n* for parts of different size *L* of the Spanish book *La Regenta*. Right: Same distributions with axes rescaled by *L* and by the corresponding size of vocabulary *V*. The data collapse is the indication of the validity of the scaling law, so, $D_L(n) = L^{-1}V^{-1}g(L^{-1}n)$, with g(x) the (unspecified) scaling function.

Biomimicri As A Method For Developing Cognitive Agents

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Anybody exposed to babies soon notices that they have a tendency to imitate individuals with whom they come into contact. Indeed this imitative behavior is one of the earliest activities of babies. For instance, Meltzoff & Moore reported an experiment in which "Newborn infants ranging in age from 0.7 to 71 hours old were tested for their ability to imitate 2 adult facial gestures: mouth opening and tongue protrusion", [1]. At least one of the explanations of this early imitation for babies less then 3 days old is that it is instrumental, geared to better interact with the care providers. It is also a general behavior of babies that can be observed across all cultures, Western and non-Western, [1]. Indeed one can assume that a 71-hour-old baby has absorbed very little or no culture. Later on, when babies begin to grow the use imitation to evaluate the consequences of actions, e.g. if a behavior or action and its consequences are rewarding, the child is very likely to imitate the same behavior or action, otherwise will stay away from it, [2], [3]. It is conceivable that both animal and human knowledge and behavior may include a concatenation of: "observation", "evaluation", "imitation", "evaluation", and "learning". Once the results of certain behavior have been shown to be good or bad, this information becomes part of what has been learned. Once a sufficient number of lessons have been learned, all these lessons become part of the animal or human toolbox to navigate through life. This is only a simplified view of the results of the studies of child development theorists, but it is a simplified model that may explain in layman language what happens. This view could help to develop manmade entities able to evolve independently in a way akin to what happens in nature. These man-made entities may take the form of software programs, of small hardware devices (e.g. robots) or both. To avoid costly mistakes we must model our man-made entities before we build them, [4]. For the purpose of modeling and simulation, structurally and architecturally simple entities can be identified with autonomous cognitive agent, [4], [5], [6]. We followed the philosophy of biomimicri because we believe that at various points in time natural evolution happened because of the actions of entities unable to deal with crisp values and unable to express computationally complex mathematical formulas, [7], [8]. We show how structurally simple agents can observe, evaluate, imitate, and iteratively evaluate & imitate and, in so doing, act to their own survival and evolutionary advantage.

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ETOS — domain specific language for discrete simulation

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Our project of domain specific language for event based discrete simulation ETOS (presented on Solstice 2013) has new goal — to become more universal platform for discrete simulation [1] by extension of SimPy [2] core by a new layer. This layer supports user specifications of shared objects providing cooperative and synchronization managers (i.e. not only competitive resource managers of classical queuing systems).

The new ETOS covers extended domain of usability for example multi-agent system simulations[3], Markov chain representation and simulation of parallel (concurrent) tasks within software applications. The new stage of ETOS system also uses upgraded syntax and semantics of our universal SIM-DSL language with new flexible and comprehensible specification of simulation parameters (based on simplified JSON objects embedded in XML attributes) and representation of oriented graphs in interconnected universal Python library. The new version preserves main advantages of ETOS system — easier cooperation of teams within simulation projects and high level of abstraction for end users.



Figure 1: Simulation of MAS in ETOS

The new support of extended shared objects is being tested in a simulation of coalition and alliance formation in multi-agents system (see Figure 1, protocol defined in [4]). The results in real world simulation will be presented.

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Behavioral and Network Origins of Wealth Inequality: Insights from a Virtual World

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The richest 1% own nearly half of all global wealth. The richest 10% claim about 86% of global wealth, so that 90% of the world's population live on a small rest. The inequity of wealth is a strong driving force in human history and has been a central subject of economics [1, 2]. Studies of the connection between wealth and social behavior are restricted to surveys or behavioral experiments, and are limited in number and scope. In this paper we use data from the massive multiplayer online game (MMOG) Pardus (www.pardus.at), where people live a virtual life in synthetic (computer game) worlds [3]. The essence of MMOGs is the open-ended simultaneous interaction of many human players. Although all goods produced and traded are virtual, the economy as such is real: players invest time and effort to produce, distribute, consume and dispose these virtual goods and services. Economical and sociological data are easily accessible in virtual worlds, which has made them a natural field for research [4, 5, 6].



Figure 1: Binned means of wealth-gain, i.e. wealth per total activity, as a function of properties of the trade network. Color represents the logarithm of the wealth-gain, from blue (lowest) to red (highest), see color bar right. Empty bins are white.

We find that the wealth distribution in Pardus has a similar shape like wealth distributions of 'real' countries, including an exponential bulk and a power-law tail. The power-law exponent of Pardus is within the range of real-world powerlaw exponents describing the moderately rich. The Gini index shows that wealth is slightly more equally distributed in Pardus than in many Western industrial countries. We observe that the shape of the wealth distribution is stable. We find that wealthy players organize in social groups and invest in their social reputation by constructive actions. Analyzing the trade network, we observe that wealthy players trade with many others (Fig. 1A), while their trade partners trade with fewer others (Fig. 1B), and hardly among each other (Fig. 1C). In the friendship and enmity networks we see that the wealthy are well respected, and show animosity – if at all – only towards public enemies.

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The Associating Lattice Gas in the Presence of Interacting Solutes

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In this work, the Associating Lattice Gas[1] in three dimensions is employed to simulate an structured solvent (like water) in the presence of polar solutes. The model is defined in a body centered cubic lattice where each site can be occupied by a solvent, a solute or remain empty. Solute and solvent interact attractively, while the solvent-solvent interaction is made directional by bonding arms, mimicking hydrogen bonds. The system's behavior was then obtained via Monte Carlo simulations in the grand-canonical ensemble, where the densities can freely fluctuate. By setting the coupling energies and the chemical potential of both, solute (μ_s) and solvent (μ_w), the phase diagrams in the plane temperature *T versus* μ_w were obtained. It was seem that, depending on the solvent-solute coupling (θ) and on μ_s several two and three phases coexistences are present[2]. These coexistences involves a) the gas (G) phase, with low densities of both particles, b) the low density liquid phase, LDL (LDLs) with solvent structured in one sublattice and low (high) solute concentration, c) the high density liquid (HDL) with solvent structured in both solute.



Figure 1: Phase diagrams: pure solvent (black) and solution (red). First (continuous lines) and second order transitions (dashed lines) and the TMD (dotted lines). (a) $\theta = -0.3$ and $\mu_s = -0.2$, (b) $\theta = -1.1$ and $\mu_s = -6$

In Fig. 1 we exhibit the phase diagram for low (a) and high (b) values of θ . LDL(s) is replaced by LA as θ rises, also changing the topology of the diagram by the insertion of a HDL-LA coexistence. The left shift in LDLs-G and right shift in LA-G are the expected behavior for non-ideal solutions where solvent-solute interactions are weaker and stronger, respectively, then solvent-solvent one.

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DNA Sequencing by Discrete Dynamics DNA Elongation Monitoring

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The one of most popular problem in modern genetics, biology and medicine is determination of the primary nucleotide sequence of the DNA of living organisms (DNA sequencing). This paper describes the label-free DNA sequencing principle, based on the observation of a discrete dynamics of DNA sequence elongation phase. The label-free DNA sequencing approach based on 4 solutions with different nucleotides (dNTP) concentration was proposed in [1]. The DNA strand contains four types of dNTP: adenine (A), cytosine (C), guanine (G) and thymine (T). Incorporation of nucleotides is performed under base pair rules, where, in DNA, G-C, and A-T (called complementary dNTP). The elongation reaction is driven by a type of enzyme, called a polymerase, which contains a reaction site. At the reaction site, the polymerase sequentially incorporates dNTP into a growing DNA chain. The order of the dNTP in the growing polynucleotide chain is governed by the DNA template and base pair rules. Also, there is the time elapses between the incorporation of one nucleotide and the incorporation of the next nucleotide ("time delay") because, as described above, incorporation do not occur simultaneously. Assuming a particular dNTP concentration, delays in nucleotide incorporation are fairly uniform, with some variability depending on diffusion dNTP molecules to reaction site. Thus, it is appropriate to speak of an "average incorporation delay". Therefore, depending upon reaction-specific factors such as reaction temperature and the concentration of a given dNTP in the solution, a elongation phase for a particular type of dNTP could have an average incorporation delay of a specific time.



Seq_i	Т	G	C	Α
Sol_C	1	8	4	5
Sol_A	9	2	4	3
Sol_T	4	2	3	7
Sol_G	4	5	9	1

Figure 1: 2D cellular automata for DNA strand growth modeling

Table 1: Table with delay times for different solutions

When the concentration in the solution, for example, adenine, will be reduced (Sol_A), the "average incorporation delay" for adenine incorporation is increasing, it will occur in DNA position with T-dNTP. The sample results for test DNA sequence "TGCA" is shown at the Tab.1. Column contains delays for each position in the sequence, and one raw for each experiment. Delay for complementary dNTP is above 6. So, particular solution type and detected long delay can uniquely define dNTP type in particular position. The dynamical model for DNA elongation based on a cellular automata (fig.1) was developed and studied by numerical simulation. The model describes diffusion process in the nucleotides solution and based on Margolus neighborhood [2]. Each automata cell contains nucleotide or can be empty. The model can simulate the elongation stage (growth strands of DNA) and dynamics of nucleotides incorporated into rising DNA strand for given parameters of DNA replication process. The model allows to estimate the "average incorporation delay" for different dNTP concentration in the solution. The paper presents estimates of concentration and experimetrs count for successful DNA sequencing. Estimates were obtained for different types of DNA sequences. The limit values for number of copied DNA sequences for required probability of nucleotide incorporation event detection and correct DNA sequence determination was obtained also.

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Multi-strategy game as a complex system

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In this study we address how the Tangled Nature model of evolutionary ecology [1] is related to evolutionary game theory [2]. To do this we study replicator dynamics with extinctions and mutations[3]. We perform numerical simulations of a game, where each player can play one of a large number of strategies. The game is defined with a payoff matrix whose elements are random numbers which can be positive or negative, with majority being zero. At the beginning of the simulation we choose randomly a small number of strategies to be played. Reproduction of players is done according to the replicator equation in which a small amount of mutations is introduced. In this way new strategies can appear in the system. Additionally we introduce an extinction threshold; strategies with a frequency less than this threshold are removed from the system. The resulting behaviour shows complex characteristics similar to those of the Tangled Nature model (see Figure). The dynamics has two types of phases: a quasi stable phase in which the number of used strategies is more or less constant and hectic phases where creation and extinct of strategies happens at a high rate. We conclude that the complex behaviour of the Tangled Nature model, which is in good agreement with observations on ecosystems [4, 5], also arrises from the game theoretic basis of the reflector dynamics. Finally we investigate various lifetime distributions and find fat tail distributions similar to those often observed for real systems[6].



Figure 1: Diversity of strategies in time. On y axes are all the possible strategies in the system and the red dot indicates that at the time step there is a non zero frequency of the players using this strategy.

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Sociophysics of Human Virtual Dynamics

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The Human Virtual Dynamics (HVD) have assumed a crucial role in modern societies, well beyond the expectations, at least of politicians around the world. HVD relies on every interaction network over different, and typical, timescales, mediated by technological environments (i.e. web base systems, ICT devices, etc). The social networks are rapidly becoming the principal autoritas even for the "ethical" and "moral" education of people, as well as the places where the "opinions", the "credencies", the "beliefs", and sometimes the "whishes" are shaped and managed. In the latest decades disciplines as sociophysics and econophysics developed models to describe the behaviour of humans, and human groups, in interaction [1]. Nowadays the modern tools developed within the Information and Communication Technology domain (ICT) allow a new and very effective setting to both, standardized and validate the sociophysical and sociopsychologycal models, and to develop a radically new approach to study the human social dynamics. Moreover a "sociophysics of virtual human dynamics" would allow to investigate the relation between the dynamics of cultures, societies and generally big communities (i.e. big data analysis), with respect to the small group dynamics (e.g. families, work and friends communities, etc.), assessing the role of mesoscopic entities on the overall dynamics interwined in social phenomena. In order to fill such a gap recent sociophysical studies introduced cognitive elements and mechanisms [2]. Such kind of model to characterize the node's dynamics, and to keep into account explicitly the evolution of the relations among people, coupled with the standard evolution of the state variable (e.g. opinion). To validate such approach we built an experimental framework to investigate the small group dynamics, exploiting a web based application in order to reach an optimal control of the experimental conditions and artefacts [3]. The basical assumption of sociophysics relies on the dependency of the state of the node (i.e. or the state of its edges), to the interactions with the others (e.g. frequently modeled as particles' collision). We started testing such hyphotesys along different experimental conditions, studying the effect of the "external field", and of the nature of the task faced by the group, on the relation between the network of communication (i.e. the contacts), the affinity among participants, and their opinion/state [4]. The results suggest that the correct approach of the sociophysical theory, assessing how for a quite short small group dynamics without any external field (i.e. baseline condition), it is possible to predict the final affinities among subject just considering the dynamics of their interactions/communication (without considering the content of the messages). Introducing a first order perturbation of the external field (i.e. a frustrated minority game), we observed a decreased linear predictability of the final state of the community just considering the interactions [5]. Within this condition we verify how the analysis of the cliques characterizing the comunicative network, still allows to predict the stability/metastability of the network dynamics. Such a predictability decrease again if the external field is perturbated introducing a polarizing topic for the discussion [6]. In this condition is possible to verify how the complexity of the interaction (i.e. the content of the messages) become relevant to predict the final state of the system. Finally we validated our affinity opinion model, comparing an empirical estimation of the model parameters, with the real cognitive characteristics (i.e. personality factors) of the participants [7]. Our data reveals an interesting correlation between one fundamental parameter of the model and a real features of the nodes' cognitive system. Moreover empirical data suggested a possible sligth modification of the standard models, introducing a repulsion dynamics coupled with the standard effect of attraction. Such a mechanism appears to increase the forecasting efficiency of the model, and cast light on the complex role of the contact network topology on the typical regime dominating the human small group dynamics.

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6th Conference Discrete Models of Complex Systems

Ordering Colors into Strings by Agents

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Initially a 2d cell field of size $n \times n$ is given that contains particles with four randomly distributed colors. Each color represents a certain property of the particle, like spin orientation. The task is to align the particles according to a global objective function by moving agents. Particles can be rearranged by magnetic fields [1] or laser beams [2]. In [5] the objective was to align to the particles' spins which are in the majority at the beginning. Here the objective is to form horizontal or vertical strings as long as possible. A horizontal string consists only of \uparrow spins or only of \downarrow spins, and a vertical string only of \rightarrow , or \leftarrow spins respectively. The idea is to optimize the conductivity of the array for electrons tunneling through the array of magnetic cells which are separated by a thin non-magnetic layer. The effect in mind is called *spin-dependent tunneling* or *giant magnetoresistance* [3]. The string length count (a measure for the conductivity) is increased by one if three spins in sequence have the same direction which is orthogonal to the string's direction. First the capabilities of the agents (actions, inputs, number of control states) have to be defined, because they decide on how effective the task can be solved at all. The used agents can perform 24 actions, combinations of moving, turning and coloring. The agents can react on 9 input situations, combinations of the own color, the color in front, the own direction, and blocking cases. The agents' behavior is determined by an embedded finite state machine (FSM, algorithm) with 6 states only. For a given 8×8 field with 16 agents an FSM was evolved by a genetic procedure based on mutation where the procedure was executed stepwise with an inreasing difficulty and an increasing number of fields in the test set. It turned out that the task is difficult to solve perfectly (maximum total string length count is n(n-3)). A simulation example with evolved agents is shown in Fig. 1. Starting from a random configuration, the agents are able to increase the string length count, thereby reaching a relative high conductivity. The whole system including the agents was modeled by cellular automata. In the implementation of the system, the CA-w model (cellular automata with write access) [4] was used in order to reduce the implementation effort and speed up the simulation.



Figure 1: The initial field at time t = 0 is colored randomly. 16 agents are moving around, thereby turning the colors (4 spin directions) in a way that preferably long strings of the same color appear. The string count *a* increases with time. Electrons can tunnel through the array more easily when they are aligned as strings of parallel spins.

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Adding New Neurons on the Tail of a Binomial

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Various hypotheses about the role of adult-born DG cells in hippocampal functions have been illustrated with simple connectionist models, but it has been challenging to assess them quantitatively with accurate network models. Yet such a quantitative assessment is critical, in view of the limited extent to which adult neurogenesis appears to occur in normal ecological conditions. For example, it would seem farfetched to consider hypothetical mechanisms that require, in order to be effective, a 50% turnover of granule cells every month, in a 1-year old rat.

A network model we have studied of the dentate gyrus as a spatial random pattern generator [1], based on the spatial activity patterns observed with single unit recording [2], enables such a quantitative assessment of the impact of adult-born dentate granule cells on the generation of CA3 spatial representations. The model shows that, given plausible values of other parameters, the information encoded in rat CA3 representations is maximal when each CA3 unit receives inputs from an intermediate number of DG units, around the value 50 reported by neuroanatomical studies. In this regime, the CA3 units which participate in a new spatial representation are those that receive strong concurrent inputs from at least (roughly) 2 DG units – effectively sampling the tail of the distribution of input strengths across CA3 units. It follows that limited additional excitability in a relatively small proportion of new DG units can have an enhanced effect, leading to distinct CA3 patterns of activity.

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Dynamical Phase Transition in the Ising model on Scale-Free Networks

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Dynamical phase transition (DPT) in the Ising model on scale-free (SF) networks under the influence of the oscillating magnetic field [1] is studied by means of Monte Carlo simulations. The transition consists in the change of the character of the hysteresis loop (the order parameter - magnetization weighted with node degrees - vs. the actual field) from symmetric for the dynamically disordered phase to asymmetric for the ordered phase as the temperature or the field parameters (amplitude or frequency) are varied. This work is an extension of Ref. [2], where this problem was studied in the case of the Barabási-Albert network with the distribution of the node degrees $P(k) \propto k^{-\gamma}$ with $\gamma = 3$; here, a more general case of SF networks with $\gamma > 2$ is investigated. For networks with different numbers of nodes N, approximate phase borders are obtained on a plane h (field amplitude) vs. T (temperature). As in the case of static ferromagnetic transition, for $2 < \gamma < 3$ the critical temperature for the DPT increases with N, while for $\gamma > 3$ there is a distinct DPT with the critical temperature which can be obtained from the crossing point of the Binder cumulants U_L for different system sizes.



Figure 1: Examples of the Binder cumulant U_L as a function of themperature T for SF networks with different γ

On the phase borders, second- and first-order DPTs occur, for the ranges of parameters separated by tricritical points. It is shown that close to these points with increasing the system size the Binder cumulant changes its character from a monotonically decreasing function of T, which is a signature of the second-order DPT, to a function with sharp negative minimum, which is a signature of the first-order DPT. Hence, the position of the tricritical point is shifted toward higher values of T and lower values of h with increasing N, i.e., the range of the critical parameters corresponding to the first-order transition is broadened. This is in contrast with DPTs observed in the Ising model on regular lattices, where in the thermodynamic limit the transition is always second-order.

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Endogenous Dynamics in Financial and Economic Systems

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The orthodox models of economics and finance assume that systems of many agents are always in a quasiequilibrium state. This (conveniently) implies that the future evolution of the system is decoupled from its past and depends only upon the exogenous (usually Brownian) forcing. However there are many human traits and societal incentives that can cause coupling between agents' behaviours thus invalidating the averaging procedures underpinning such equilibrium models.

We use an agent-based framework, based around the idea of moving thresholds [1], that can be used to test the stability of equilibrium solutions to the presence of potentially dis-equilibrating endogenous effects. Each agent *i* is in one of two states $s_i = \pm 1$ (ie bullish or bearish in a financial setting) and will occasionally switch between them. The rules governing the switchings are easily capable of representing the findings of behavioural economics, perverse incentives, or various technical trading strategies. Changes in the aggregated 'average sentiment' $\sigma = \frac{1}{M} \sum_{i=1}^{M} s_i$ add an extra endogenous term component into the dynamics. In the continuum limit $M \to \infty$ this is represented by the usual Itô SDE for the log-price *p* modified by an additional endogenous term

$$dp = a dt + b dB + \kappa d\sigma$$

The ratio $\kappa/b > 0$ quantifies the relative strength of endogenous versus exogenous effects.

First we show that incorporating herding/contagion effects does indeed destabilize the usual Brownian asset pricing model [2]. At plausible parameter values endogenous 'boom-bust' dynamics are generated whereby a long and gradual mispricing phase is abruptly ended by a cascading process [1]. The resulting fat-tailed price change statistics are consistent with those observed in real markets.

Similar dynamics are observed when the contagion effect is replaced by a simple momentum trading strategy. Now an agent who switched to state +1 at time t^* will change back to state -1 when the price falls by a specified amount from its maximum since t^* (as the agent now perceives a downward trend). Similarly, the agent will switch back to state +1 when the price rises by a specified amount above the minimum since the latest switching. In this case it is possible to treat the market as a network of Prandtl-Ishlinskii operators whose response function to any input can be easily specified [3].

Under further mild assumptions the system in this second case can be rigorously analyzed — in particular the fattailed distribution of price changes can be computed. Furthermore, there is a critical value of the parameter κ beyond which a system-wide cascade is guaranteed to occur.

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Model Of A Population Of Autonomous Simple Cognitive Agents And Their Performance In Various Environments

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Autonomous robots are intelligent machines exhibiting a predefined behaviour, such that, once they are deployed, they can perform tasks by themselves (autonomously), without human intervention, or if required with minimal human intervention. For the purpose of modeling and simulation, structurally and architecturally simple autonomous robots can be identified with autonomous cognitive agents. A cognitive agent is an abstraction of an autonomous entity capable of interacting with its environment and other agents [1, 2, 3]. With the goal in mind of possible hardware implementation, there is an obvious interest in identifying the simplest possible architecture still capable of producing meaningful results for the desire task. In this context we study a problem of defining autonomous cognitive agents capable of learning from and adapting to their environment and providing results in a multi-agent setting. In the presented work we develop cognitive agents, which we call naïve creatures, able to operate in a multi-agent and multi-species agent reality and capable of surviving by learning the dangers of the universe of the experiment and of developing a simple strategy of survival, as a species. We present an extension of the works [4, 5]. We describe our model of a population of autonomous simple naïve creatures experiencing fear and/or desire learning to cross a highway, and their experimental virtual universe. We investigate how these feelings and creature mobility along a highway may affect the creatures' ability to learn to successfully cross the highway. We present selected simulation results and their analysis for various types of highways and densities of car traffic.

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Reconstructing network structure from dynamical signals

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Two key factors determine the functioning of any complex system: interactions among the units and the topology of inter-unit connections [1]. While detecting properties of interactions between two units/nodes is often achievable with adequate experimental equipment, reconstructing the topology of a potentially very large real network is a more challenging task, which typically requires domain-specific approaches [2]. On the other hand, theoretical reconstruction concepts are based on paradigmatic dynamical models such as phase oscillators [3], some of which have been experimentally tested. We hereby propose a new method of network reconstruction from the dynamical time series, relying on the novel concept of derivative-variable correlation. Using a tunable observable as a parameter, the reconstruction of any network with known interaction functions is formulated via simple matrix equation [4, 5]. We suggest a procedure aimed at optimizing the reconstruction from the time series of length comparable to the characteristic dynamical time scale. Our method includes a way to reliably estimate the reconstruction precision, via errorbars associated with the link weights, as illustrated in Fig. 1. Our method is also robust to model error (mismatches in the knowledge of the interaction functions) and observation errors (noisy measurements of the dynamical time series).



Figure 1: Elements (link weights) of the original adjacency matrix for some dynamical network (circles), and the best reconstruction obtained with our method (crosses). The the corresponding errorbars are shown. Model error and observation error scenarios in (a) and (b), respectively.

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Non-equilibrium Phase Transitions in the Brain

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I shall briefly describe recent studies in our group of mathematical models for brain cooperative functions and network structure. They focus on phenomenology such as the propagation of weak signals competing with noise and the spontaneous process of synaptic pruning during early human growth. I plan to show how the combination of familiar concepts in physics such as those of chaos, non-equilibrium, phase transitions and criticality provides a coherent understanding of some of the brain complex behaviour. The following graphs and caption comments illustrate some aspects of my talk.



Figure 1: Input-output correlation function corresponding to a weak signal transmitting in the presence of noise, as a function of the noise level, showing stochastic resonances that can be associated with non-equilibrium phase transitions.



Figure 2: Left, the phase diagram (showing the section: synaptic short-time noise versus grade of synchronization) corresponding to a Hopfield model in which synapses undergo different levels of fatigue or depression (parameter Φ) and only a fraction of neurons (parameter ρ) are synchronized at each time. Different phases here correspond to different qualitative behaviours. Some of these behaviours are illustrated in the graphs to the right.

Interacting Scales and Coupled Phenomena in Nature and Models

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Interacting time and space scales are universal. They frequently go hand in hand with coupled phenomena which can be observed in nature and man-made systems. Such mutiscale coupled phenomena are fundamental to our knowledge about all the systems surrounding us, ranging rom such global systems as the climate of our planet, to such tiny ones as quantum dots, and all he way down to the building blocks of life such as nucleic acid biological molecules.

In this talk I will provide an overview of some coupled multiscale problems that we face in studying physical, engineering, and biological systems. I will start from considering tiny objects, known as low dimensional nanostructures, and will give examples on why the nanoscale is becoming increasingly important in the applications affecting our everyday lives. By using fully coupled mathematical models, I will show how to build on the previous results in developing a new theory, while analyzing the influence of coupled multiscale effects on properties of these tiny objects.

In the remaining time, I'll talk about coupled multiscale problems in studying biological structures constructed from ribonucleic acid (RNA). As compared to deoxyribonucleic acid (DNA) and some other bio-molecules, RNA offers not only a much greater variety of interactions but also great conformational flexibility, making it an important functional material in many bioengineering and medical applications. Examples of numerical simulations of such biological structures will be shown, based on our developed coarse-grained methodologies.

Structural properties of complex networks

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Many complex systems, both natural [1], and man-made [2][3], can be represented as multiplex or interdependent networks. Multiple dependencies make a system more fragile: damage to one element can lead to avalanches of failures throughout the system [4][5]. Recent theoretical investigation of two [6] or more [7]networks in which vertices in each network mutually depend on vertices in other networks has shown that indeed small initial failures can cascade back and forth through the networks, leading to a discontinuous collapse of the whole system. Damage in one network propagates along edges and leads to damage in the other network. This is an individual stage of a cascade in back-and-forth damage propagation. Son et al. showed that this approach can be simplified and is equivalent to considering damage propagation in multiplex networks. They proposed a simple mapping between the model used in [6] in which a vertex in one network has a mutual dependence on exactly one vertex in the other network, and a multiplex network with one kind of vertex but two kinds of edges. The mapping is achieved by simply merging the mutually dependent vertices from the two networks.



Figure 1: A small network with two kinds of edges (left). Applying the algorithm described in the text non-viable vertices are removed leaving two viable clusters (right).

In this talk I will revisit a number of well-studied problems concerning structural properties of complex networks. Some concepts like percolation, k-core organization, bootstrap percolation and avalanche collapse of the giant viable component in multiplex networks are well well-known to the audience but I will present them in a different perspective showing the recent analytical advances from a network theory point of view. In contrast, we study the avalanches of damage triggered by the removal of randomly chosen single vertices. These avalanches increase in size approaching the critical point, signaling the impending collapse of the giant viable cluster. At the critical point the mean avalanche size diverges. Below the transition, on the other hand, there is no precursor for the appearance of the giant viable cluster. The transition is thus asymmetric. I will show that however different problems they share some common features like a hybrid phase transition.

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Agent-Based Modeling and Social Structure in Bloggers' Dynamics

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Emotions play pivotal role in both offline and online social dynamics. Although, collective emotional behavior of users is frequently observed in online societies [1, 2, 3], the role of emotions in online communication and their connection with emerging social structure of online communities are still not thoroughly understood.

In this paper, we study mechanisms underlying the collective emotional behavior of Bloggers by using the agentbased modeling and the parameters inferred from the empirical data of popular BBC Blogs and discussion-driven Diggs [4]. Agents, whose individual emotional states are described by their valence and arousal, are embedded in bipartite network of users and posts. This bipartite network evolves trough the addition of agents and their actions on posts; agents transfer their current emotional state to post by posting an emotional comment. Emotional state of agent fluctuates in time as a direct consequence of indirect interaction with other agents trough its ego-network of posts. We show that the indirect communication of the emotion in the model rules, combined with the action-delay time and the circadian rhythm extracted from the empirical data, can explain the genesis of emotional bursts by users on popular Blogs and similar Web portals.

Our results show that the emotion-driven dynamics leads to long-range correlations and emergent networks with community structure, also observed in analysis of empirical data [1, 2]. We show that the size and activity of evolving agents communities correlates with the expression of negative emotions (critique), see Figure 1.



Figure 1: Time series of the number of comments posted by the agents belonging to a given community (left), and the charge of these comments (right).

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Bargaining with discrete strategies

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Imagine two players having to share a sum of money. One proposes a split (p), and the other can either agree with it or not (q). No haggling is allowed. If there is an agreement, the sum is shared according to the proposal. If not, both players remain empty handed. This is the blueprint of the ultimatum game [1]. Seminal experiments on ultimatum bargaining have revealed that humans are remarkably fond of fair play [2]. When asked to share something, unfair offers are rare and their acceptance rate is small. Traditionally, the ultimatum game has been studied with continuous strategies, and it has been shown that empathy and spatiality may lead to the evolution of fairness [3]. However, evolutionary games with continuous strategies often hide the true complexity of the problem, because solutions that would be driven by pattern formation are unstable. Discrete strategies in the ultimatum game open the gate to fascinatingly rich dynamical behavior. The highly webbed phase diagram presented in Fig. 1, featuring both continuous and discontinuous phase transitions as well as a tri-critical point, reveals the hidden complexity behind the pursuit of human fair play [4].



Figure 1: Phase diagram for five discrete empathetic strategies $E_{0...4}$ in the presence of strategy A, which is characterized by the parameters p and q. Solid red and dashed blue lines denote continuous and discontinuous phase transitions, respectively. Besides several single and two-strategy phases, a rich array of three-strategy phases, in part governed by intricate cyclic dominance, can be observed. For further details see [4].

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Complexity and the evolution of music-production networks

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According to the composer Arnold Schönberg [1] our listening habits are determined by two opposing forces, the desire for variety and the demand for uniformity in music. We quantify these notions by constructing music production networks connecting music styles with musical instruments. We study the evolution of these networks from 1969 to 2010. We extract the similarity network of styles and this network shows clusters of music styles allowing characterize them by instruments. Complexity of a music style will be determined by the amount of variation and uniformity [2]. We find an inverse relation between variety and uniformity being stable during the last fifty years. However, individually music styles undergo dramatic changes in their complexity over time.



Figure 1: Variety $V(s,t_f)$ and uniformity $U(s,t_f)$ for music styles with at least 50 records within the time-span $t_f=2004-2010$. The music styles fall almost on a curved line where variety and uniformity are inversely related. "Experimental" is the music style with the highest variety of instrumentation, styles with lowest variety and highest uniformity belong to the "electronic" and "hip hop" genres.

We show that such dramatic changes in the complexity of a music style can be related to its sales number and to the number of artists a particular music style attracts. As a music style increases its number of records its variety increases due to the number of musicians attracted to the style. At the same time the uniformity decreases. On the other hand, album sales increase by increasing uniformity and decreasing variety. We can interpret this dynamics as a "formula of success" of the mainstream industry.

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Vogel-Fulcher freezing in relaxor ferroelectrics and dipolar glasses

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Relaxor ferroelectrics (relaxors) are random displacive systems such as substitutionally disordered perovskite oxides, in contrast to dipolar glasses (DGs) which can be regarded as randomly diluted order-disorder type ionic solids. In both cases several common features are observed, for example, a broad temperature peak in the ac dielectric susceptibility, a splitting between the ac and the quasistatic field-cooled susceptibility, and a broad distribution of relaxation times characterized by a Vogel-Fulcher (VF) type divergence of the longest relaxation time, i.e., $\tau = \tau_0 exp[U/k(T - T_0)]$, where T_0 is the VF freezing temperature. It is now widely recognized that the elementary degrees of freedom in relaxors are the so-called polar nanoregions (PNRs), which are formed at relatively high temperatures and are characterized by possessing reorientable dipole moments of variable lengths. In dipolar glasses, however, the dipoles have a fixed length and are thus analogous to magnetic spin glasses, however, with the addition of random electric fields. It has been suggested by that the mechanism leading to the VF freezing in relaxors is the growth and percolation of PNR clusters as the temperature is lowered [1].

Here we present a semi-phenomenological model of relaxation based on the Landau-type free energy for the polarization p of the medium in which the PNRs are embedded, and assume a linear coupling between p and the PNR polarization P(r). We show that when the 4th-order Landau coefficient is negative (b < 0) the medium is correlated with the PNR, and the correlation radius r_c , which is a measure of the PNR size, depends on the temperature T and the applied electric field E. As T is lowered or E increased, r_c increases and the volume fraction η occupied by the cluster of PNRs starts to grow. As η reaches the percolation threshold $\eta_p \sim 0.3$, the PNRs form an "infinite" cluster and the time necessary for overturning the cluster diverges according to a modified VF law with a field-dependent freezing temperature $T_0(E)$ [2]. The predicted E-dependence agrees qualitatively with experiments in relaxors PMN-PT [3] and PLZT [4].

When b > 0, however, the medium remains uncorrelated with the PNRs and a different mechanism is needed. This is the case of DGs, where the elementary degrees of freedom are individual dipoles for which the Adam-Gibbs mechanism of cooperative rearrangement of molecules in glass forming liquids applies, again leading to the VF relaxation time [5]. This allows us to formulate a phenomenological criterion, which can be used to discriminate between the relaxor state (b < 0) and the analogous DG state (b > 0).

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Interacting particle systems: Integrability vs. universality

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Stochastic models of interacting particles attracted a lot of attention as exactly solvable models sharing the universal behaviour of the Kardar-Parisi-Zhang (KPZ) and Edwards-Wilkinson (EW) universality classes. Special mathematical structure of integrable systems makes plenty analytic results available. Among them are universal distributions and correlation functions. The first simplest models having been solved are the asymmetric and symmetric simple exclusion processes, which were used as a paradigmatic examples for KPZ and EW universality classes respectively. Both these models were solved by the Bethe ansatz technique, which is the basic method of solving the integrable models.

Though the simple exclusion processes allow probing into main features of the KPZ and EW universal behaviour it is desirable to include various types of interactions into the dynamics to see whether the universality is stable against the modification of the dynamics. However not all interactions are consistent with exact solvability. Integrability imposes strict limitations on the dynamical rules. Therefore it is of primary interest to find as general as possible model, which would preserve the integrability property.

Another important property that has long been recognized to be shared by many exactly solvable stochastic particle models is the simple structure of traslationally invariant stationary measure having a form of product of one-site factors. This allows for complete characterization of the stationary correlations by the use of the toolbox of equilibrium statistical mechanics, developed for systems with non-interacting degrees of freedom. In the talk we show how to obtain the most general three-parametric interacting particle model, which possesses both the product stationary measure and the Bethe anstaz solvability. This model includes the asymmetric simple exclusion process as well as many other models as a limiting cases. We give a brief review of the particular models that can be obtained from the general model, some of which were studied before and some are new, and discuss different types of universal and non-universal behaviour exhibited by the model at different values of parameters.

Quantifying self-organization and complexity with a wavelet machine?

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Statistical complexity is an unbiased property that may be evaluated from data grassberger[1]. Computational mechanics, a methodology for detection and quantifying patterns, uses the so called ε -machine representation of a stochastic process whose algebraic structure captures symmetries of the process under study[2]. An ε -machine requires the least number of model components to represent the structures in the process. and from the memory of the process, one can obtain the entropy production and the structural complexity of the system. The ε -machine is visually represented as a directed graph where the nodes are the causal states of the process and edges reflect transition probabilities between causal states in successive time-steps. Causal states may represented as a spatio-temporal stochastic patterns of cellular automata as shown in [3]. Recently, we have developed a *w*-machine (*w* stand for wavelet) in analogy with the ε -machine, which is a versatile method for quantifying complexity that at the same time determines the optimal wavelet for capturing self-organization of the dynamic system and which performs superior denoising[4]. The method is based on a parametric model for a wavelet tree distribution attributing hidden Markov (HM) variable to each node of the tree. The wavelet tree is considered as a self-organizing system by identifying hidden states of the wavelet coefficients with local causal states.

The local complexity in the wavelet-domain is determined as a function of scale and the global complexity of the tree is utilized as an optimality measure for the decomposition. The local statistical complexity of a spatio-temporal process is defined as the information (Shannon) entropy of the local causal state. The *w*-machine posseses the property of approximate unifilarity indicating that the knowledge of the current state and measurement implies no uncertainty in the next state.

We illustrate the method and its advantages on several types of data including fluid turbulence and paradigmatic dynamic systems, and we also mention other possible uses.

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Micro and Macro Benefits of Random Investments in Financial Markets

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In this paper, making use of statistical physics tools, we address the specific role of randomness in financial markets, both at micro and macro level. In particular, we will review some recent results obtained about the effectiveness of random strategies of investment, compared with some of the most used trading strategies for forecasting the behavior of real financial indexes. We also push forward our analysis by means of a Self-Organized Criticality model, able to simulate financial avalanches in trading communities with different network topologies, where a Pareto-like power law behavior of wealth spontaneously emerges. In this context we present new findings and suggestions for policies based on the effects that random strategies can have in terms of reduction of dangerous financial avalanches, in a community of traders with a small-world structure, changes from a power law to an exponential curve by introducing a small percentage of random traders in the network.



Figure 1: Distributions of the absolute values of the size of herding avalanches occurring in a small-world (SW) community of investors, with and without random traders, for the case of the FTSE MIB index . Each curve has been cumulated over 10 different events. In the absence of random traders, (circles), the distributions follow a well defined power law behavior. On the other hand, increasing the amount of random traders, in particular with percentages of 5% (squares) and 10% (triangles), the distributions tend to become exponential.

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Topological bifurcations in a model of a society of reasonable contrarians

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People are often divided into conformists and contrarians, the former tending to align to the majority opinion in their neighborhood and the latter tending to disagree with that majority. In practice, however, the contrarian tendency is rarely followed when there is an overwhelming majority with a given opinion, which denotes a social norm. Such reasonable contrarian behavior is often considered a mark of independent thought, and can be a useful strategy in financial markets.

We present the opinion dynamics of a society of reasonable contrarian agents. The model is a cellular automaton of Ising type, with antiferromagnetic pair interactions modeling contrarianism and plaquette terms modeling social norms. We introduce the entropy of the collective variable as a way of comparing deterministic (mean-field) and probabilistic (simulations) bifurcation diagrams.

In the mean field approximation the model exhibits bifurcations and a chaotic phase, interpreted as coherent oscillations of the whole society. However, in a one-dimensional spatial arrangement one observes incoherent oscillations and a constant average.

In simulations on Watts-Strogatz networks with a small-world effect the mean field behavior is recovered, with a bifurcation diagram that resembles the mean-field one, but using the rewiring probability as the control parameter. Similar bifurcation diagrams are found for scale free networks, and we are able to compute an effective connectivity for such networks.

Network growth model with intrinsic vertex fitness

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A class of network growth models with attachment rules governed by intrinsic node fitness is investigated. Both the individual node degree distribution and the degree correlation properties of the network are obtained as functions of the network growth rules. We find analytical solutions to the inverse, design, problems of matching the growth rules to the required (e.g., power-law) node degree distribution and more generally to the required degree correlation function. We find that the design problems do not always have solutions. Among the specific conditions on the existence of solutions to the design problems is the requirement that the node degree distribution has to be broader than a certain threshold and the fact that factorizability of the correlation functions requires singular distributions of the node fitnesses. More generally, the restrictions on the input distributions and correlations that ensure solvability of the design problems are expressed in terms of the analytical properties of their generating functions.

Fitness based network composition has been introduced in Ref. [2]. These networks, which are build by static intrinsic vertex fitness are of particular interest because of the information amount that each node is assumed to have. Unlike in the classical model of preferential attachment [1], where each arriving node must have complete information about the geometry of the entire network, in the fitness model each node must have knowledge about a non-topological quantity. This weaker assumption about the accessible information is realistic in many scenarios. Consider for instance the case of investment networks, where the number of investors is usually not disclosed, but information about intrinsic quality of different funds is available.

The fitness based network literature is classically separating between the distribution of fitness and an attachment kernel that translates the fitness of a pair of nodes into the probability that this pair shares an edge. We illustrate that this separation is not necessary and that it increases the number of degrees of freedom for statistical analysis without gaining additional information. If fitness is defined as a normalised rank order of some node intrinsic characteristic, then the fitness distribution becomes a constant and everything can be expressed in terms of the rank order.

At the end of the talk, more recent work about failure spreading on fitness based networks will be discussed. The classical failure-percolation model of Watts [3] is expanded to account for heterogeneous resilience inside the network. Some of the insights are illustrated in Fig. 1.



Figure 1: Size of the vulnerable component for different settings. (a) Power-law distributed fitness leads to a more robust network. (b) Mutual attractiveness induces more robustness than random selection. (c) Increasing the density of the network increases its stability.

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From Wilson-Cowan to Kuramoto: Multiplex Formulation of Neural Activity

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In our work we elucidate the connection between mesoscopic models of neural activity (i.e. involving neural populations of size $\sim 10^9$) and macroscopic models describing whole-brain dynamics ($\sim 10^{11}$ neurons) from a network perspective. We start from a multiplex network of weakly coupled Wilson-Cowan oscillators [1] with explicit time delays: Each node is associated with a distinct brain region and carries a two-dimensional oscillatory state with fixed period describing the local averaged activities of excitatory (E) and inhibitory (I) subpopulations within that region. Each link is associated with a structural connection between adjacent regions and is dynamically represented by a coupling function of weak magnitude with explicit time delays (associated with synaptic transmission delays). By applying a generalized form of the Malkin theorem for weakly coupled oscillators [3], we show that this model is equivalent to a Kuramoto-type phase model [2], where the time delays are transformed into phase shifts and the four types of interactions (E-E, E-I, I-E and I-I) correspond to different layers of a multilayer network.



(a) Synchronization as a function of coupling and phase shift



(b) Power spectra for different phase shifts at critical coupling

Figure 1: Global effects of a time delay-induced phase shift on neural oscillations (see text below)

Furthermore, empirical facts about the synaptic architecture of the brain (mainly concerning the ratio and distribution of excitatory and inhibitory neurons) allow us to reduce the four-layer model to two layers, one (E-E) being the ordinary Kuramoto model and the other (E-I) being a phase-shifted Kuramoto model with phase shift δ . In both layers, the coupling strength has the same value K. In this reduced two-layer model, we observe two global dynamical effects as shown in Figure 1 above: In Figure 1(a) it is depicted how synchronization - as measured by the order parameter r which takes values between 0 (unsynchronized state) and 1 (synchronized state) - is affected both by the coupling strength K and the phase shift δ . Figure 1(b) shows that the mean power spectrum of all oscillators peaks at increasing values with increasing phase shift δ at critical coupling strength. Both features correspond to physiological effects related to inhibitory control of neural activity in the brain: drugs designed to prevent epileptic seizures (anticonvulsants) may also enhance gamma oscillations.

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Stock Price Dynamics: Application of Simple Fluids Models and Percolation

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For two decades, a new interdisciplinary field called econophysics has emerged by applying models and concepts associated with statistical physics to economic and financial phenomena [1]. Substantial effort is focused on analysis and modelling of financial time series, whose non-trivial features are called empirical stylized facts [2]. Those are typically scaling behavior, fat-tailed price change distributions, short-time negatively correlated price change, long-time correlations in absolute returns, absence of autocorrelation in return and volatility clustering. Various models including percolation models [3, 4, 5] have been introduced in order to reproduce and explain them. The present work has been inspired by the above mentioned.

In the present work we use simple fluids models (hard-sphere fluid, square-well fluid, Lennard-Jones fluid and their two-dimensional versions as well) in order to get clusters of particles representing clusters of traders. We carry out common Metropolis Monte Carlo simulations in a canonical ensemble [6]. We use various bond criteria to define a cluster and determine the corresponding percolation threshold [7]. Then there are several parameters to adjust (e.g. system density, trading activity) in order to obtain data (e.g. probability distribution of returns, autocorrelation function and the Hurst exponent in dependance of the time lag) that characterize some of the important features of the empirical data (we use the data from the Prague Stock Exchange for this comparison).

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A Structural and Functional Network as a Tool to Analyze Complex Biological Systems

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At the protein level, it is a challenge to differentiate between direct physical interactions and functional associations, which do not involve direct atomic contacts between macromolecules [1]. The information retrieved from the protein interfaces obtained by atomic-resolution of protein complexes, represents an invaluable source in order to built-up the "structure-based" biological networks. In this work, we exemplified this concept on the kallikrein-kinin (KKS) and renin-angiotensin (RAS) [2]. The later represent two highly regulated proteolytic systems which participate in several physiological and pathological processes i.e. cardiovascular and renal homeostasis, growth and development and inflammation [3]. To gain insight into the multilayered interaction of the KKS-RAS systems, a "structural" protein network was built up on the 3D domain-domain interactions [2]. The essential domains that link these systems are: Cystatin, Peptidase_C1, Thyroglobulin_1, Insulin, CIMR (Cation-independent mannose-6-phosphate receptor repeat), fn2 (Fibronectin type II domain), fn1 (Fibronectin type I domain), EGF, Trypsin, and Serpin. We found that the CIMR domain is located at the core of the network, thus connecting both systems. From the later, all domain interactors up to level 4 were retrieved, thus displaying a more comprehensive representation of the KKS-RAS structural network. Moreover, a "functional network" based on several 'omics' tools was built up (Fig. 1). A signalling network of 104 proteins led to 1574 non-redundant protein-protein interactions, where 72 significant complexes were identified. In conclusion, this integrative approach provides a new framework to analyze complex biological systems.



Figure 1: Functional network of the kallikrein-kinin (A) and renin-angiotensin (B) system

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New Numerical Solutions of Newtonian Three-body Problem: Scaling and Regularities

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For two centuries, attempts were made at a general solution to the Newtonian three-body problem, until H. Bruns showed that only specific particular solutions were possible. Yet only three families of collisionless periodic orbits were known until recently. Presently, systematic numerical searching for periodic solutions has become possible. In [1], we showed 13 new periodic orbits, and in [2] we found 11 more. We used topological method based on the shape-sphere projection to classify and identify orbits [3].



Figure 1: Negative logarithm of the return proximity function (left) and one of the periodic solutions (right)

Furthermore, we use all presently known planar collisionless periodic three-body orbits with vanishing angular momentum to study the three-body version of Kepler's third law: we found that the scaling regularities are related to orbit's topological property on the shape sphere. This fact can be used to predict properties of several classes of as yet undiscovered orbits.

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Triggering Mechanisms in Emotion Dynamics: From Brain Activity to Collective Social Behavior

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In human conduct, emotions play an important role starting from the brain dynamics of each individual to social interactions and aggregated group behaviors. Thus, the dynamics of emotions [1] appears as a subject of interdisciplinary research. Quantitative study of emotions in psychology was made possible by Russell's model where an emotion is determined by numerical components in a multidimensional space [2]. To recognize an emotion as it is known in common life, at least two components are necessary, arousal and valence, measuring the degree of reactivity and attraction or repulsion. According to recent developments in the science of affective computing, these components of emotion can be extracted from a written text [3]. In social neurology, traditional techniques of monitoring the brain functions (EEG,MEG,fMRI) are now applied to capture signals from brains of people during a communication process [4].



Figure 1: The ineraction patterns in online social network MySpace shows dominance of positive emotion (red links).

In this work, applying methods of statistical physics [5], we describe the appearance of collective emotional behavior in online social networks. We use agent-directed simulations where agents exchange emotional messages along the network's links; the dynamic variables, arousal and valence, characterize the agent's state, whereas high arousal triggers an agent's action. We determine several quantitative measures that indicate clustering of events with emotional contents. The focus is on statistics of the influence fields that trigger emotional action of an individual agent in the network. Further, we examine the effects of random or (emotionally) coherent external inputs to these triggering fields at individual agent level and to the emergent collective dynamics.

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Entropies for Complex Systems

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Shannon and Khinchin built their foundational information theoretic work on four axioms that completely determine the information-theoretic entropy to be of Boltzmann-Gibbs type, $SBG = -\sum_i p_i \log(p_i)$. For non-ergodic systems the separation axiom (Shannon-Khinchin axiom 4) is not valid. We show that whenever this axiom is violated—as is the case in most complex systems—entropy takes the more general form,

$$S_{c,d} \propto \sum_{i=1}^{W} \Gamma(d+1, 1-c\log(p_i))$$
, (1)

where c and d are characteristic scaling exponents, and Γ is the incomplete Gamma function. The exponents (c,d) parametrize equivalence classes which precisely characterise all (!) interacting and non-interacting statistical systems in the thermodynamic limit [1], including those that typically exhibit power laws or stretched exponential distributions. This allows us for example to derive Tsallis entropy (as a special case) from solid first principles. Further we show [2] how the knowledge of the phase space volume of a system and the requirement of extensivity allows to uniquely determine (c,d). We ask how the these entropies are related to the 'Maximum entropy principle' (MEP). In particular we show how the first Shannon-Khinchin axiom allows us to separate the value for observing the most likely distribution function of a statistical system, into a 'maximum entropy' (log of multiplicity) and constraint terms. Remarkably, the generalized extensive entropy is not necessarily identical with the generalized maximum entropy functional. In general for non-ergodic systems both concepts are tightly related but distinct [3].

We demonstrate the practical relevance of our results on path-dependent random walks (non-Markovian systems with long-term memory) where the random walker's choices (left or right) depending on the history of the trajectory. We are able to compute the time dependent distribution functions from the knowledge of the maximum entropy, which is analytically derived from the microscopic update rules. Self-organized critical systems such as sand piles or particular types of spin systems with densifying interactions are other examples that can be understood within the presented framework.

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A simple one-dimensional model for composite polymer knots

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Knots are known to affect the physical properties of polymers [1, 2, 3, 4], as well as the functionality of biopolymers such as DNA and proteins [5, 6]. Furthermore, several recent studies brought under the light the relevance of knots in nanotechnological applications [4, 7, 8, 9].

It is possible, and frequent, for several knots to appear on the same chain, which is then said to host a *composite knot*; in fact, it has been mathematically proved that such configurations are by far the most probable for long polymers [10, 11]. In spite of their ubiquity, only a few studies focused on composite knots, and their behavior remains largely unexplored. One of the few standing points in the physics of composite knots is that, in the limit of long polymers rings, their knotting probability tends to the product of the knotting probabilities of the single factor knots composing them. This factorization of the knotting probability has been justified with the assumption that in long polymers knots become localized and therefore behave like point-like decorations on the rings [12, 13].

Here, using Monte Carlo simulations and advanced knot localization methods, we analyze the length and distribution of prime components in composite knots tied on Freely Jointed Polymer Rings. For increasing contour length, we observe the progressive factorization of composite knots into separated prime components. However, we observe that a complete factorization, equivalent to the "decorated ring" picture, is not obtained even for rings of contour lengths up to tens of times the most probable length of the prime knots tied on the rings.

Following our results, we suggest that the "decorated ring" hypothesis may not be necessary to explain the factorization of the knotting probabilities, at least when polymers excluded volume is not relevant. We rationalize the behavior of the system through a simple one dimensional model in which prime knots are replaced by sliplinks randomly placed on a circle, with the only constraint that the length of the loops has the same distribution of the length of the corresponding prime knots.

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Influence of the grid resolution on output accuracy and parameter sensitivity

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Belgian chocolates have an excellent reputation on the international market. However, the whitish haze formed over time on the surface of chocolate, known as fat bloom, poses a worrisome problem hampering the export of these products [1]. Therefore, there is a need to develop better models that combine mass transfer with the phase behavior for accurately predicting the migration of liquid fat and the occurrence of fat bloom [1]. The authors developed a 2D stochastic cellular automaton (CA) based model to describe the migration of liquid fat (from the filling) to the surface, after which this model was parametrized using an experimental time series of data [2]. The inverse problem of retrieving the values of the four model parameters of the CA's transition function corresponding to the experimental data, was solved by a grid search of the parameter space, where the sum of absolute errors (SAE) served as a goodness of fit measure. A square grid \mathscr{G} was used, which represents of a vertical cross-section of the system wherein fat migration is studied. By presuming the side length of a square cell, Δx , to be 0.0001 m, 50 rows and 260 columns of cells are needed to model the real system from which the experimental data were obtained. The value of Δx is the result of a trade-off. On the one hand, setting Δx as large as possible is desired to reduce the computation time of the simulations. On the other hand, a small enough grid resolution and therefore small enough Δx is wanted to prevent overly sensitive model parameters that result in very fluctuating solutions from simulation to simulation.

Figures 1(a)–1(c) show the results of the influence of the grid resolution on the accuracy of the simulated outcome as well as the speed of the calculations for different grid resolutions. It can be seen that although the total number of grid cells decreases, the goodness of the fit between experimental and simulated time series stays more or less the same (cf. SAE). Further, as expected, it is clear that the lower number of grid cells substantially decreases calculation times. On the other hand, this increase in calculation speed comes at a price when looking at the standard deviation, σ . The latter implies that although the calculations go faster when the grid resolution is smaller, the results fluctuate much more from simulation to simulation. Further, the influence of the grid resolution on the parameter sensitivity is studied through the use of the Elementary Effects method. Although a clear trend is difficult to discern due to the stochasticity of the model for the three grids with the highest resolution, it is clear that once below a certain threshold resolution, in this case clearly for the resolution of 20×104 , the parameter sensitivity doubles to triples. The latter signifies that small deviations from an optimal value for the parameters may result in larger differences of the simulated output.



Figure 1: Influence of grid resolution on (a) SAE, (b) standard deviation and (c) calculation time.

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6th Conference Discrete Models of Complex Systems

Understanding the Large Scale Urban Vehicular Mobility by Discrete Models

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Urban vehicular traffic congestion is an increasingly serious problem that is significantly affecting many aspects of the quality of metropolis life around the world [1]. Local governments of large cities are under heavy pressure to find large amounts of financial spending for continuously testing the capacities of city roads, and making new adjustment and plan to the existing transportation infrastructures, in order to increase the capacities of cities' transportation systems [2]. Critical issue for transportation systems is how to efficiently use the existing road network systems and the information collection systems for vehicular movements and distributions to reduce traffic congestion and travel delays as well as to further save energy consumption and to improve safety [3]. The main problem here is handling the vehicular dynamics within the capacity of the existing road system by predicting and guiding the vehicular traffics. Therefore, effective and accurate real-time understanding of the traffic parameters, such as traffic volumes, speeds, occupancies, etc., are needed [4]. However, these vehicular dynamic parameters are formed by individual vehicular mobilities.

In this talk, I will first introduce our proposed microscopic-level discrete models to describe the individual mobility behavior precisely, and macroscopic-level discrete models to characterize the gross quantities or metrics, by treating the traffic according to fluid dynamics and, therefore, can reveal the large-scale overall vehicular mobility behaviors and traffic patterns. Specifically, we explore the use of an open Jackson queueing network to model the macroscopic level vehicular mobility. Our proposed simple model can accurately describe the vehicular mobility and, moreover, it can predict various measures of network-level performance, such as the vehicular distribution, and vehicular-level performance, such as average sojourn time in each area and the number of sojourned areas in the networks. Model validation based on two large scale urban city vehicular motion traces confirms that this simple model can accurately predict a number of system metrics crucial for vehicular network performance evaluation.

On the other hand, focusing on investigating how much the vehicular mobility can be predicted, I will talk about the prediction limitations described by discrete entropy model, to answer the fundamental questions of what is the role of the randomness playing in the human/vehicular mobility, is there any regularity in the daily vehicular movement, and to what degree is the mobility predictable. By using two large-scale urban city vehicular traces of *Beijing* and *Shanghai*, we propose an intuitive but effective model of areas transition to describe the vehicular mobility among the areas divided by the city intersections. Based on this model, we examine the predictability limits of large scale urban vehicular networks and derive the maximal predictability based on the methodology of entropy theory. Our study finds that about 78% to 99% of the location and 70% of the staying time, respectively, are predicable. Our findings thus reveal that there is a strong regularity in the daily vehicular mobility, which can be exploited in practical prediction algorithm design.

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Enhancing network functionalities by manipulating complex networks

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Complex network theory offers us a novel way to characterize and understand real systems with high complexity. Meanwhile, it also allows us to control real systems by manipulating the corresponding networks. Network manipulation includes a wide range of issues ranging from structural changes in networks to the adjustment of dynamical processes on networks. Related procedures on networks are usually associated with a cost constraint, i.e. network topology cannot be arbitrarily modified and the dynamics on networks cannot be completely redesigned. In our works, we find that in many cases relatively small manipulations of the networks can lead to significant improvement of the network functions. In this presentation, I will focus on manipulation on network structures: removing spurious connections from networks to increase their reliability [1], swapping links in infrastructure networks to improve their robustness against both link and node attacks [2], and assigning direction to links in undirected networks to enhance network synchronizability [3].

Removing spurious links from networks is crucial for improving the reliability of network data. Many similaritybased methods can be used for this problem. The basic idea is that a link connecting dissimilar nodes is likely to be a spurious one. The accuracy of these methods are usually high. However, if links are removed based on these methods, the giant component will be destoryed and the networks properties change significantly. This is because some links connecting different communities of the network are removed. The solution is to design a hybrid method combining the similarity index and edge-betweenness index. With our method, the detection accuracy is high and the size of the giant component is preserved.

Another aspect of the network reliability is its robustness against malicious attack. Previous works have already pointed out that scale-free networks are very robust against random failure, but very sensitive to target attack. This is because the network will break into pieces if some large degree nodes are removed. Recently, it was pointed out that the scale-free networks can also resist large degree node attack if the network forms an onion structure. However, we find that the onion structure is even less robust than normal scale-free networks against link attack. Accordingly, we designed a link robustness index based on edge-betweeness. By optimizing it, we obtained a network structure tolerant of malicious link attack.

The final work aims to enhance network synchronization by assigning directions to the links in undirected networks. In the literature, an effective method called Residual Degree Gradient method was proposed to assign link directions by decomposing networks. Though it can improve synchronization, we find such method may lead to serious synchronization failure. We thus introduce a method called Residual Edge-betweenness Gradient method to avoid synchronization failure. Simulation shows that our method significantly outperforms the existing one.

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