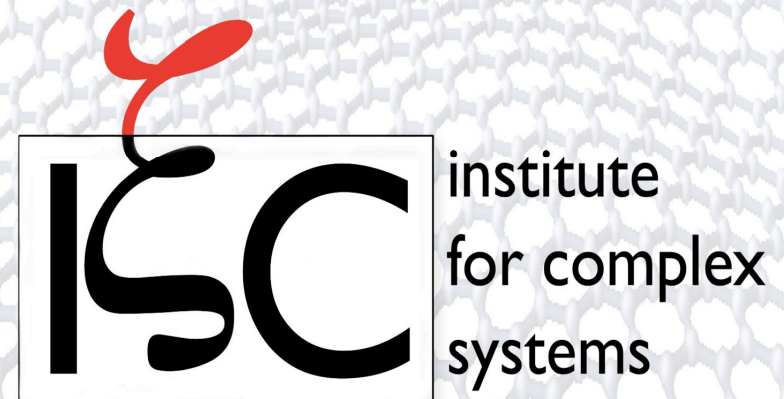


Physics of Complexity @ ISC

November 2015



National Research Council of Italy

Physics of Complexity @ ISC

The **Institute of Complex System** (*ISC*) of the National Research Council (*CNR*) was created in 2004.

The science of complexity studies the emergence of collective properties in systems with a large number of interacting elements. These elements might be atoms in a physical context or say macromolecules in a biological one, but also individuals or companies in a socio-economic context.

Focusing on the structure of the interconnections and the general architecture of systems, the science of complexity departs from the traditional approach based on individual components.

Rome, November 2015

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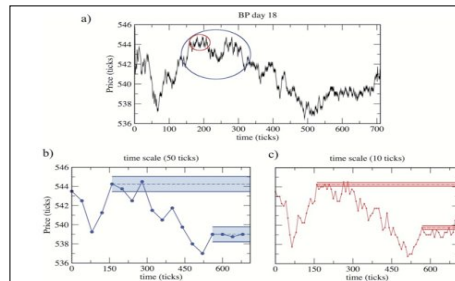
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keywords

- *Complex Networks*
- *Agent Based Models*
- *Financial time series*

Agent based models represent an alternative to the standard economic theory, which assumes perfect rationality and information. The consequences of the relaxation of these assumptions can be studied by numerical simulations in which traders buy or sell stocks in a virtual financial market, following personal or collective strategies. These models can reproduce the main statistical features of price dynamics.

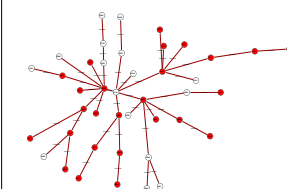


Concepts and tools borrowed by statistical mechanics and complexity can be used to investigate the properties of **financial time series**. Recently we have shown that non trivial memory effects are present in the price dynamics of stocks [1] and that extreme events lead to a power law relation between skewness and kurtosis, that is valid also for the statistics of earthquakes [2].

[1] Garzarelli et al. *Scientific reports* 4 (2014).

[2] Cristelli et al. *Physical Review E* 85.6 (2012): 066108.

Is there a common path on countries' development, or each country must follow his own way? In order to produce cars, one has to learn before how to produce wheels? The theory of **complex networks** can be applied to answer these questions and describe the industrialization of countries. Starting from the empirical data about the worldwide exports we have built a network of products that are connected by a directed link if there is a causality relationship between them. We can suggest paths in the product space which are easier to achieve, driving countries' policies during their industrialization.



Zaccaria et al.
"How the taxonomy of products drives the economic development of countries." *PloS one* 9.12 (2014): e113770.



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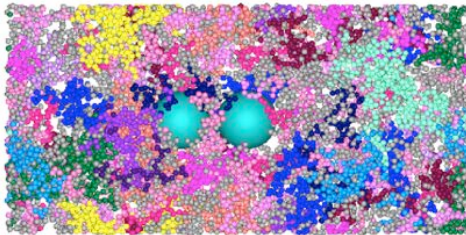
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keywords

- *Simulation and theory of soft matter systems*
- *Gel and glass transitions*
- *Complex effective interactions: novel phases and anomalous dynamics*

Complex effective interactions

Colloidal particles can be treated as super-atoms moving in a continuum (solvent) in the framework of statistical mechanics. They interact with *effective potentials* that can be tuned arbitrarily by changing the properties of the particle (e.g. shape, architecture, heterogeneous surface) or by varying externally the conditions of the solutions in which they are suspended. In this way, they experience interactions and show phenomena that are not found in atomic or molecular systems.

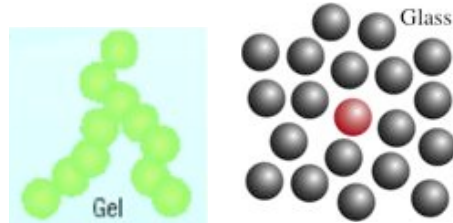


The simplest way to control the interactions between colloids is to add smaller particles (cosolute) in the solution, which originate so-called depletion interactions. By tuning the properties of the co-solutes, novel effects can be found. For example a co-solute close to its percolation transition induces so-called Casimir-like forces on the colloids.

N.Gnan, E. Zaccarelli, F.Sciortino *Nature Communications* 5, 3267 (2014)

Gels and Glasses

By tuning effective interactions, we find not only new thermodynamic phases (e.g. crystals with unconventional lattice spacings) but also different types of disordered arrested states: **Gels** where particles are organized into networks and **Glasses** where particles are blocked by their neighbours.



Recently, we discovered equilibrium gels formed by patchy particles, which were experimentally observed in colloidal clays. This work, done in collaboration with ISC experimental researchers B. Ruzicka and R. Angelini, has also revealed the possibility of other unconventional glasses with partially frozen orientational degrees of freedom (R. Angelini, E. Zaccarelli, F. de Melo Marques, M. Sztucki, A. Flueraşu, G. Ruocco and B. Ruzicka, *Nat. Comm.* 5, 3267 2014).

Nowadays we are working on microgel particles, made by crosslinked polymer networks, which are thermo-responsive to elucidate the nature of their arrested states at ultra-high densities.



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keywords

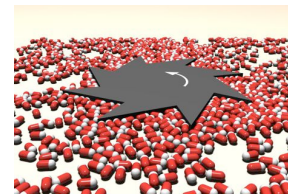
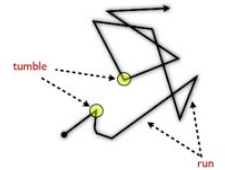
- *Active matter*
- *Self-propelled particles*
- *Modeling and simulations*

Active Matter – Motile bacteria

Ensembles of animate organisms, such as motile *E.coli* bacteria, behave in a very rich and surprising way if compared to inanimate objects, such as atoms or molecules in a liquid. By converting chemical energy into mechanical motion, active suspensions represent a very interesting class of out-of-equilibrium systems, giving rise to complex pattern formation and spatio-temporal behaviors.

Run-and-tumble dynamics

Bacterial motion can be described as a simple run-and-tumble walk, consisting in a straight line motion at constant speed (*run*) interrupted by a random reorientation of the swimming direction (*tumble*). The resulting dynamics (telegrapher's like equation of motion) can be analyzed in different contexts (external fields, escape problems).

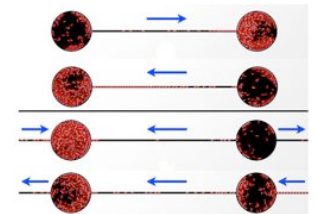


Shaped and passive objects in bacterial baths

Shaped objects or colloidal beads immersed in a bacterial bath experience "active" forces, giving rise to rectification phenomena and effective interactions. For example, asymmetrically shaped gears perform unidirectional rotational motion when immersed in a bath of self-propelled microorganisms.

Active particles in confined geometry

Swimmers dynamics is strongly influenced by boundaries. Self-propelled bacteria confined in micro-chambers connected by thin channels spontaneously generate flow currents giving rise to self-sustained density oscillations.





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keywords

- *Soft Matter: experiments*
- *Gel and glass transition*
- *Structure and dynamics of disordered systems*

Gel and glass transition in soft matter systems

Recent advances in the study of soft matter have led in the last decades to a better understanding of equilibrium and non-equilibrium states and to the discovery of new phases besides the ones commonly experienced in atomic or molecular systems. In the wide panorama of soft materials, an important role is played by colloidal suspensions that offer the possibility to observe unusual phase diagrams including reentrant or empty liquid regimes [1], multiple arrested states, such as gels and glassy states and glass-glass transitions [2]. My work is focused in particular on charged colloidal clays and more recently on colloidal microgels. The experimental work is developed, in collaboration with Dr. B. Ruzicka, in our laboratories at Sapienza University, through dynamic light scattering (DLS), differential scanning calorimetry (DSC) and rheometry and in collaboration with Dr. E. Zaccarelli for comparison with theory and simulations.

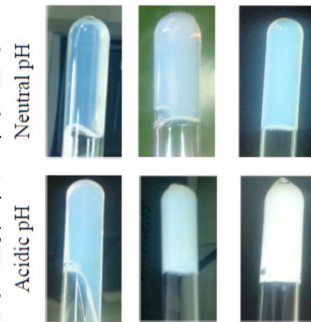


Fig.: Arrested state of an interpenetrated polymer network colloidal microgel obtained by increasing temperature.

[1] *Nat. Mater.* **10**, 56 (2011).

X-rays scattering scattering to probe structure and dynamics of soft matter

Soft matter systems exhibit complex behavior involving a broad range of length and time scales. For this reason, alongside laboratory techniques such as DLS, rheometry and DSC, synchrotron-based methods are powerful tools to extend their study and understanding over such wide spatial and temporal scales. This part of my work is developed mainly at the European Synchrotron radiation facility (ESRF) in Grenoble through X-ray photon correlation spectroscopy and small angle X-ray scattering techniques and complemented with neutron scattering measurements.

[2] *Nat. Commun.* **5**, 4049 (2014)

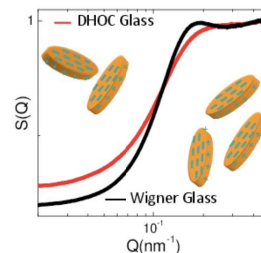


Fig.: Static structure factor of a colloidal clay, Laponite, across the glass-glass transition [2].



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keywords

- *Collective Behavior in Biological Systems*
- *(Non-Equilibrium) Statistical Mechanics*
- *Inference, Modeling & Simulations*

From bird flocks to fish schools, from insect swarms to cell colonies, collective behaviour is a very widespread phenomenon in many biological systems. It is hard to define, but easy to recognize. What are the mechanisms regulating collective behaviour in biological systems?

The aim of my work is to understand the collective behaviour exhibited by flocks of starlings (*Sturnus vulgaris*) and swarms of non-biting midges (*Chironomidae*) through the analysis of synchronized high speed image sequences from three cameras. Using stereo matching and other computer vision techniques, we are able to reconstruct, in three dimensions, the trajectories of individual animals within the aggregation. Further analysis of the trajectories should lead to a better understanding of the fundamental interaction rules between individuals.

- *Information transfer and behavioural inertia in starling flocks*
Nature Physics **10** (9), 691-696

- *Interaction ruling animal collective behavior depends on topological rather than metric distance: Evidence from a field study*
Proceedings of the National Academy of Sciences **105** (4), 1232-1237

- *Collective Behaviour without Collective Order in Wild Swarms of Midges*
PloS Computational Biology **10** (7), e1003697

Experiments find coherent information transfer through biological groups on length and time scales distinctly below those on which asymptotically correct hydrodynamic theories apply.

We need a new continuum theory of collective motion coupling the velocity and density fields to the inertial spin field recently introduced to describe information propagation in natural flocks of birds.

- *Silent Flocks*
arXiv:1410.2868



Which is the "recipe" that exactly reproduces the real biological systems? Which are the hypotheses cut by the "Occam's Razor" for which "entities must not be multiplied beyond necessity"?

Biological data have hidden information to be gathered: we have to solve the "Inverse Problem". We can try to take advantage of the critical aspects of biological systems because in physics this is synonymous of phase transition and scale invariance. A deeper statistical mechanics insight allows us to "rescale" biological data from different events and obtain more robust and meaningful answers. It is required a complex and interdisciplinary line of research that includes:

- Deep theoretical expertise on statistical physics of complex systems ;
- Bayesian inference on biological data;
- Optimization - Simulations - Modeling ;

- *Scale-free correlations in starling flocks*
Proceedings of the National Academy of Sciences **107** (26), 11865-11870

- *Statistical mechanics for natural flocks of birds*
Proceedings of the National Academy of Sciences **109** (13), 4786-4791



Ruggero Vaia

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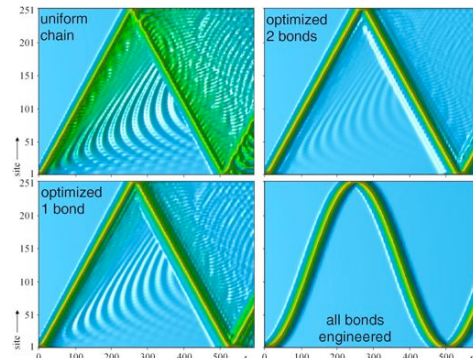
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keywords

- Theory of low-dimensional magnetic systems
- Optimal transport in one-dimensional quantum and classical channels
- Quantum effects in low-dimensional systems

Transport in 1D channels

At variance with their continuous case, one-dimensional arrays are intrinsically dispersive: an injected wavepacket is not faithfully transmitted, but loses its coherence. However, if the array's bonds (i.e., spring constants, hopping amplitudes,...) are properly tuned, dispersion can be limited or even eliminated. This is relevant, e.g., in the case of the transfer of quantum states between distant qubits, which is one of the basic tasks that a quantum computer based on qubits located on fixed positions has to accomplish. Obtaining *perfect transmission* is theoretically possible at the cost of tuning all the systems bonds, a problematic task for a real experiment. An analysis of the transport mechanism leads to the concept of *quasi-perfect transmission*, that can be reached to high degree by only acting on few extremal bonds. The space-time evolution of a propagating excitation injected in the first site of a $N=250$ -site open array is shown in the figure: the optimization of just two bonds at the chain ends, $j_1=2N^{-1/3}$ and $j_2=1.6N^{-1/6}$, leads to an efficiency that is still larger than 98.7% in the large N limit. The same optimization problem is more complicated for a classical system.



A quantum Newton's cradle

The proposal consists in a system of atoms with two internal states trapped in a one-dimensional tube with a longitudinal optical lattice; the atoms are maintained in a strong Tonks-Girardeau regime at maximal filling. A localized endpoint disturbance of the wave-function propagates along the chain in analogy with the propagation of momentum in the classical Newton cradle. The quantum traveling signal is generally deteriorated by dispersion, e.g., for a chain with uniform bonds and is known to be zero for suitably engineered bonds, but the latter is hardly realizable in practice. Starting from these opposite situations it has been shown how the coherent behavior can be enhanced with minimal experimental effort.



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keywords

- Granular materials
- Soft matter
- Econophysics

Granular materials and Soft matter

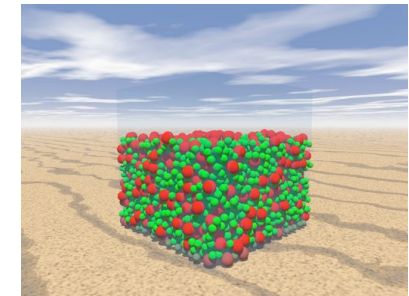
I work together with Dr. Alberto Petri and Dr. Andrea Baldassarri on the subject: friction in granular matter.

We have developed a Molecular-Dynamics code in order to simulate an assembly of grains under shear (see picture right).

Our approach follows the ones of Cundall&Strack., Massimo Pica Ciamarra et al., Silbert et al.

We are currently investigating the microscopic and macroscopic properties of granular friction, together with a thorough analysis of the stick-slip motion which takes place.

I have also worked in the past on Soft matter subjects as mixtures of colloids and polymers and ferrogels.



Econophysics

Since 2014 I have been working together with Dr. Alberto Petri and Dr. Giorgio Pontuale on the study of country-product matrix exports.

We are investigating the type of the statistical distributions which take place in these flows and the properties of export flows.



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keywords

- *Neutron spectroscopy*
- *Dynamical models of fluids*

Microscopic static and dynamic structures in disordered systems

The microscopic structural and dynamical properties of fluids are a key topic in statistical mechanics of condensed-matter many-body systems, in the whole range comprising simple monatomic and molecular gases and liquids, non-simple liquids like hydrogen-bonded fluids, conducting fluids (liquid metals), semi quantum and quantum liquids. In these systems we have been investigating both single-particle and collective phenomena.

From the experimental side, we apply neutron diffraction and neutron spectroscopy techniques. The accompanying non-trivial data analysis is conducted jointly with various kinds of simulation methods.

The most important results of the last few years are:

- a theoretical analysis based on the reformulation of fit models, leading to the full understanding of dispersion curves for collective excitations, and to a general exact relation between decay times of memory functions and lifetimes of the spectral modes;
- a theoretical analysis of time correlation functions of operators in many-body systems, proving their general property of being described as infinite series of exponential functions corresponding to the eigenmodes of the frequency spectrum;
- the development of optimized multidimensional Monte Carlo integration methods for evaluation of multiple scattering in inelastic scattering experiments;
- the analysis of ab initio simulations in parallel with experimental data on liquid-metal microdynamics, leading to the determination of some types of unified features, shown to be common to all classes of fluids, in contrast with the current point of view that involves different theoretical models;
- the analysis of quantum simulation for liquid hydrogen, deuterium, and hydrogen isotopic mixtures, leading to the assessment of non-Gaussian behaviour in the single-molecule dynamics of quantum Boltzmann fluids.



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keywords

- *Open Quantum Systems*
- *Quantum Information and Computation*
- *Low-dimensional magnetic systems*

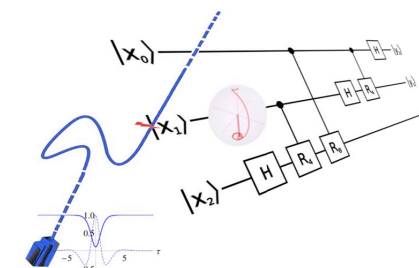
Dynamics of open quantum systems

The first step in the study of physical phenomena is that of identifying the system upon which to focus the attention, usually referred to as the "principal system". What is left out might yet contain parts that significantly affect the process under analysis, and combine to define the "environment". Quantum systems with an environment generally go under the name of Open Quantum Systems (OQS).

The core problem in studying OQS is that of considering how principal system and environment communicate and interplay during the quantum evolution induced by their mutual interaction. In fact, due to correlations that dynamically set up between the two subsystems, their respective dynamics not only stops being unitary, but it also gets a memory that wipes out markovianity even in the absence of random processes or phenomena otherwise needing a statistical approach. In fact, it is just the entanglement, i.e. the most genuinely quantum type of correlation, that mediates the information exchange between principal system and environment, insofar causing non-markovianity to emerge as a striking feature of the principal system's evolution, and one of the pivotal issues in the theory of OQS dynamics.

In this general framework we specifically concentrate our attention upon these cases:

- 1) When the environment is a many-body quantum system:-> **Quantum communication.**
- 2) When the environment is an apparatus:-> **Quantum measurements and control.**
- 3) When the environment is a complex system:-> **Finite-temperature quantum effects** in thermodynamic, chemical, and possibly biological processes.



Spin chains in quantum communication

Quantum devices are eclectic objects whose architecture varies greatly depending on their specific purpose and, perhaps primarily, on the way they are physically realized. However, there are some basic requirements that are most often assumed, amongst which the possibility of initializing the input quantum register, which implies that of individually addressing, and possibly manipulating each single qubit. When solid-state implementations are considered, with qubits embodied in the spin degrees of freedom of molecules embedded in crystalline matrices or deposited on layered substrates, individual qubit addressing can be obtained by conveying a signal through a functional wire, as qualitatively shown in figure. In particular, we study schemes where **the wire is modeled by a spin-chain** (i.e. by a one-dimensional magnetic system) and proper **signals are embodied in magnetic solitons** (i.e. in nonlinear excitations of spin chains), known for being localized, both in space and time, and robust against perturbations, which guarantee that each signal will travel down to the qubit without distortion.



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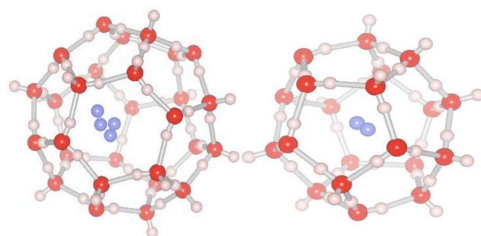
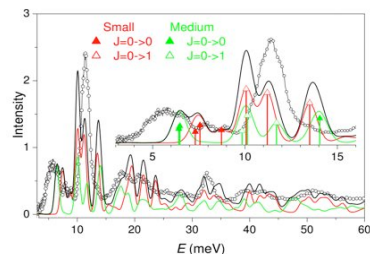
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keywords

- Hydrogen storage, clathrate-hydrates
- Materials at high pressure, Diamond Anvil Cell
- Neutron scattering, Raman and Infrared spectroscopy

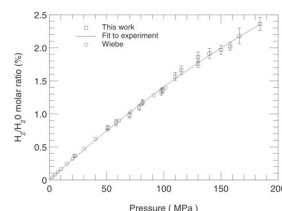
Hydrogen Clathrate Hydrates

Clathrate-hydrates are solid compounds made of water and other “guest” molecules, which are trapped in polyhedral cavities (cages). They are ubiquitous in nature. We synthesize **hydrogen clathrate-hydrates** (having different structures) in the laboratory, using a pressure higher than 1 kbar. These compounds are important for hydrogen storage but we are interested also in the quantum dynamics of the hydrogen (H_2 , D_2 or HD) in the cage, which we study with **Neutron** or **Raman spectroscopy**. The spectrum of the excitations comprise molecular **rotations**, center-of-mass quantum excitation (**rattling**) and all possible **combinations** of these. Position and intensity may be calculated with quantum codes, and compared with neutron experiments. An example for HD is in figure.



Hydrophobic Solvation

Hydrophobic gases have very low **solubility** in liquid water. In solid clathrate, hydrogen/water ratio is about 25 %. Preliminary to the study of hydrogen clathrate formation from the H_2 - H_2O liquid solution, we have studied, by means of **Raman scattering**, the solubility and the spectroscopic features of the H_2 molecule in water up to 3000 bar. It increases with pressure, but it never reaches values similar to those obtained in clathrates.



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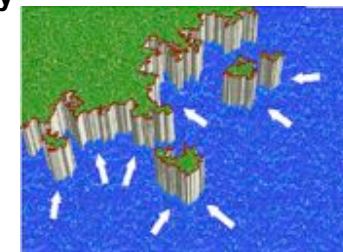
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keywords

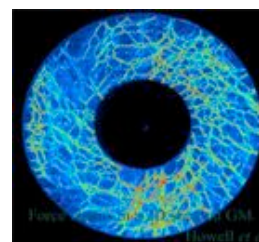
- Percolation
- Granular materials
- Stochastic processes

Rocky coast erosion and percolation theory

As shown by a minimal numerical model, percolation theory can be used as a guide to decipher the physics of rocky coast erosion and could provide precise predictions to the statistics of cliff collapses. I'm interested in possible applications of percolation theory in geomorphology, as revealed by irregular geometries or anomalous statistics.



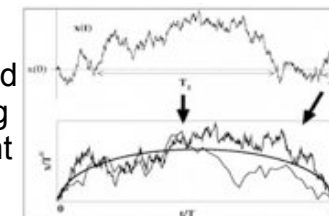
Friction in granular materials



Friction is a very old, but still open field of research, relevant from the physics at nano-scale to earthquakes. The friction response of a granular material could be very fluctuating, due to the anomalous stress propagation in the material. This systems represent an interesting laboratory, both experimentally and theoretically, for the introduction of new models and concepts.

Avalanche dynamics and crackling noise

Irregular, bursty dynamics can be modeled via simple stochastic processes, revealing unexpected connections between different physical systems (crackling noise).





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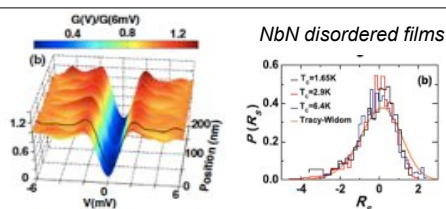
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keywords

- Theory of Many-Body Systems
- Superconductivity in low dimensions
- Materials with Novel Electronic Properties

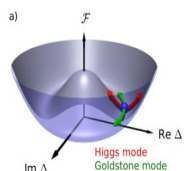
The understanding of the electronic properties of **complex solid-state systems**, where one observes the **competition** between different phenomena, requires to develop and implement a modern quantum-field theory approach. This includes several analytical techniques, ranging from a conventional perturbative expansion to the derivation of the quantum functionals for the collective degrees of freedom



The inhomogeneous local DOS measured by STM shows an universal probability distribution of the local SC order parameter when properly rescaled

A typical example of competing states is provided by **strongly disordered superconductors**: here disorder tends to order the charge, by localizing the electrons, and pairing tends to order the global electronic phase, i.e. to form the superconducting state. As a compromise, the system develops an intrinsic inhomogeneous phase with unusual glassy properties.

G.Seibold et al. Phys.Rev.Lett.108, 207004 (2012).
G. Lemaire et al. Phys. Rev. B 87, 184509 (2013).



Schematic representation of Amplitude (Higgs) and phase (Goldstone) modes in superconductors

T. Cea et al. Phys. Rev. Lett. 115, 157002 (2015).



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keywords

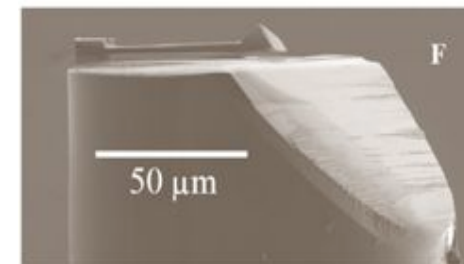
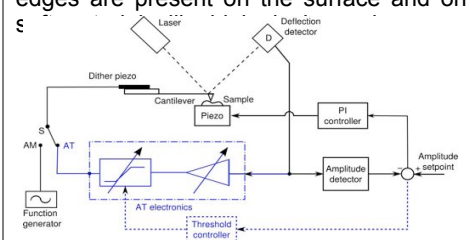
- Atomic Force Microscopy
- Biophysics
- Applied physics

Atomic force microscopy

Since its invention in 1986, AFM, has been widely used for investigating material characteristics at nanoscale level, and its improvement has rapidly led to reliable instrumentation. Although, after more the twenty years new imaging methods are still under investigation to improve image quality and speed, new probes sound more physical property of the sample and the fields of application are still growing. For example a new kind of probe fabricated by carving a cantilever at the end of a fiber is capable to detect forces and optical tunneling signals at the same time.

Self-driven cantilever oscillation

A non-linear control of cantilever oscillation amplitude dynamically adjust the gain of the self-sustained vibration of the cantilever. This new dynamic mode improves scan speed and image accuracy it results particularly effective when sharp edges are present on the surface and on ϵ



Diffusion of two molecular species in a crowded environment.

Diffusion of two fluids is studied in the frame of differential equations derived from a well defined microscopic model where crowding and steric interference are taken into account. The experiment of two ink drops simultaneously evolving in a container filled with water shows that molecular crowding results in the formation of a dynamical barrier that prevents the mixing of the drops. This phenomenon is successfully captured by the model.





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keywords

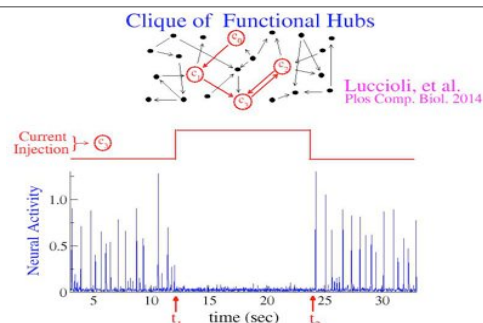
- *Nonlinear Dynamics*
- *Computational Neuroscience*
- *Synchronization*

Computational Neuroscience Lab

<http://neuro.fi.isc.cnr.it/>

The lab is active in Florence since 2006 and it is presently composed of 2 permanent researchers, 3 post-docs and 2 PhD students. The studied subjects range from the dynamics of single neurons, to the emergence of collective activity in neural networks to data analysis of neural time series, mainly spike time series. The group has published more than 50 scientific articles in the last 8 years and it has been supported by research fundings for more than 1 million euros in the last 4 years obtained from the European Union, the Italian Ministry of Foreign Affairs (MAE), the German Max-Planck-Gesellschaft, and the Italian Ministry of University and Research. The group maintains active international collaborations with the following institutions: University of Aarhus (Denmark), Ecole Normale Supérieure, Paris (France), University of Bonn (Germany), Tel Aviv University (Israel), University Pompeu Fabra, Barcelona (Spain), University of Aberdeen, University of Bristol, Imperial College London (UK), University of Michigan, University of California San Diego (USA). The Lab is the Italian hub of the Joint Italian-Israeli Laboratory in Neuroscience (2010-2019) supported by MAE.

Luccioli, Olmi, Politi, Torcini PRL (2012)
Mikkelsen, Imperato Torcini PRL (2013)



Synchronization

Synchronization is an ubiquitous phenomenon observable in many fields of science ranging from fireflies populations to neural systems, from electrical power-grids to fish banks. Our aim is to analyze such a phenomenon from the point of view of out-of-equilibrium statistical mechanics and by employing tools originating from nonlinear dynamics. Recently we addressed the problem of the synchronization of two populations of phase oscillators with inertia, discovering new peculiar dynamical states: **Chaotic Chimeras**. These states display a broken symmetry where one population is fully synchronized, while the other population is chaotic. Furthermore these states have been observed experimentally in coupled mechanical pendula.

M. Baer, E. Schoell, A. Torcini, Angew. Chem. Int. Ed (2012)
Olmi, Martens, Thutupalli, Torcini PRE (2015)



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keywords

- *Many-Body Interactions and Theoretical Physics in Condensed Matter*
- *Superconductivity and collective phenomena*
- *Graphene and low-dimensional systems*

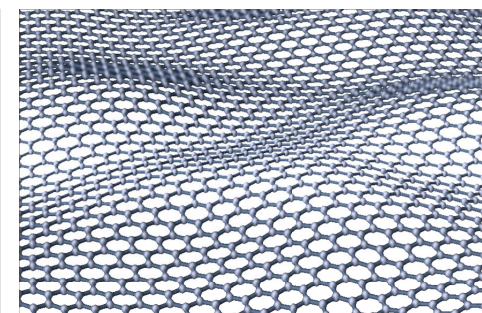
My research activity investigates the appearance of many-body phenomena of fundamental physics in a variety of specific condensed matter systems. Examples of open research lines where Master theses are available:

Graphene and post-graphene compounds

Theoretical modelling of electronic, lattice, thermodynamical, optical, and magnetic properties of two-dimensional materials (graphene, dichalcogenides,...).

Interactions and Pairing in Iron-based Superconductors and recently discovered H_3S

Microscopical description of the scattering and pairing mechanisms in the normal state (transport, optical properties) and in the superconducting state (gap symmetry).



Lattice/spin polarons and Interplay between electron-lattice and magnetic interactions
Mechanisms and properties of complex objects (*polarons*) where different degrees of freedom (electron, lattice deformation, spin) are entangled at a local scale. Itinerant vs. trapped states.

Spontaneous broken-symmetry phases in layered compounds
Nematic, charge and bond-density-waves driven by Hubbard-Hund interactions in layered two-dimensional materials.



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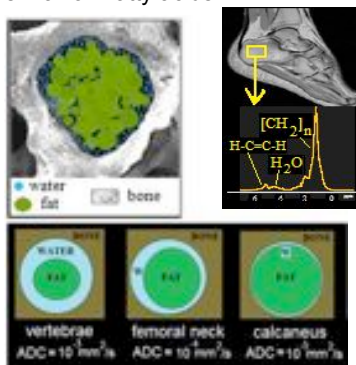
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keywords

- Nuclear Magnetic Resonance Imaging
- Anomalous diffusion in porous systems and biological tissues
- Applied physics: Medical Physics and Cultural Heritage

Osteoporosis diagnosis

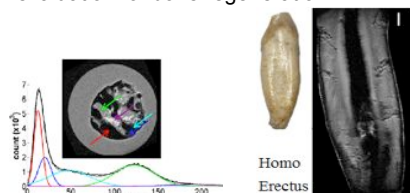
by diffusion of water in cancellous bone and spectroscopic quantification of bone marrow fatty acids.



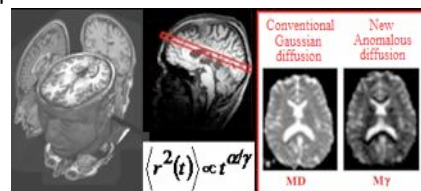
S. Capuani, Microp.Mesop.Mater 2013;178:34
S. Capuani et al. BioMed Res Intl 2015; 948610
M. Rebuzzi et al. BONE 2013;57:155-163
G. Manenti et al. BONE 2013;55:7-15

Micro MRI

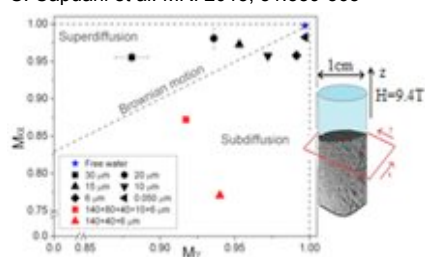
Fossil teeth, Root
3D evaluation of bone regeneration



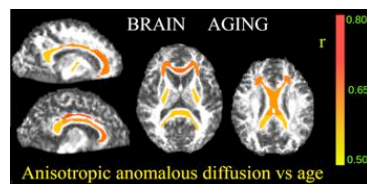
Non Gaussian diffusion of water in porous material and human brain tissues



S. De Santis et al. MRM 2011;65(4):1043.
S. Capuani et al. MRI 2013; 31:359-365



M. Palombo et al. JCP 2011;135,034504
M. Palombo et al. Sci Rep 2013;3:2631



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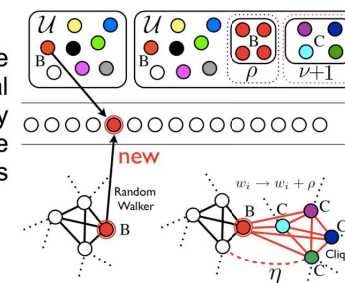
keywords

- Opinion Dynamics, Quantitative Linguistics
- Citizen Science and Human Computation
- Learning Dynamics

The dynamics of correlated novelties

Novelties are commonplace in daily life. They are also fundamental to the evolution of biological systems, human society, and technology. By opening new possibilities, one novelty can pave the way for others in a process that Kauffman has called "expanding the adjacent possible".

F. Tria et al., Sci.Rep. 4, 5890 (2014)



Web-based social computation

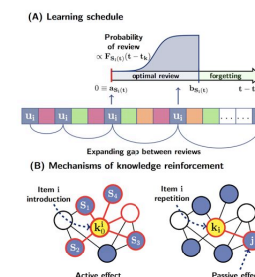


<http://www.xtribe.eu>

The Web has progressively acquired the status of an infrastructure for social computation allowing researchers to coordinate the cognitive abilities of human agents by steering the collective user activity towards predefined goals. This general trend is triggering the adoption of web-games as a very interesting laboratory to run experiments whenever the contribution of human beings is crucially required for research purposes.

Statistical modeling of learning paths

Each sphere of knowledge could be depicted as a network of correlated items. By properly exploiting these connections, innovative and more efficient learning strategies could be defined, possibly leading to a faster learning process and an enduring retention of information.





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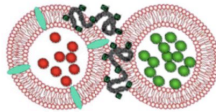
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keywords

- Self-assembly and aggregation in colloidal systems
- Supramolecular structures
- Biological cell membranes and model membrane systems

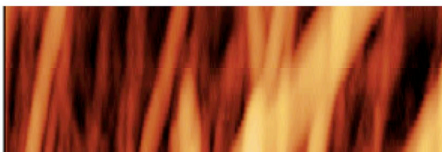
Polyelectrolyte-induced aggregation of colloidal particles

By a combined approach involving dynamic light scattering, electrophoresis and microscopy techniques, we investigate the self-assembly phenomena occurring in co-suspension of oppositely charged polyelectrolytes and colloidal particles, as lipid vesicles (liposomes), yielding the formation of a stable cluster phase, where aggregates show a novel nano-scaffolded multi-compartmental structure. Fundamental research on particle-polyion interaction and cluster aggregation mechanisms are accompanied with applicative studies aimed to develop the high potential of this system in bio-nanotechnology, as innovative drug-delivery system, in a strongly interdisciplinary ambit.



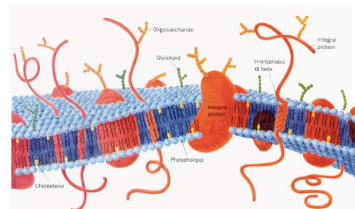
Supramolecular structures

Novel classes of biological or synthetic amphiphiles and peptides gives rise to supramolecular structures formed by hierarchical self-assembly. By controlled tuning of the physico-chemical parameters of the system, shape and dynamic transition may be observed. Macroscopically extended and robust networks due to gelation phenomena may form, whose interesting properties open the way to application as new materials in tissue engineering.



Biological and model membranes

By means of Langmuir trough, AFM and optical microscopy, we study the structural properties of cell membranes and model membranes systems, as lipidic mono and bilayers and giant vesicles, with the aim to characterize their organization with respect to environmental parameters and interactions with biological macromolecules, as drug, proteins or DNA.



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keywords

- Interdisciplinary applications of statistical physics
- Complex networks
- Dynamics of social systems

Statistical physics approach to social dynamics

In recent years it has become widely recognized that many large-scale phenomena observed in social systems are the "macroscopic" emergent effect of the "microscopic" behavior of a large number of interacting agents. This has led to the introduction of elementary models of social behavior (opinion dynamics, cultural and scientific evolution, language change). Many of these models are relatives of models that are studied in modern statistical physics, and it is natural to approach them using the same concepts and tools successfully applied in physics.

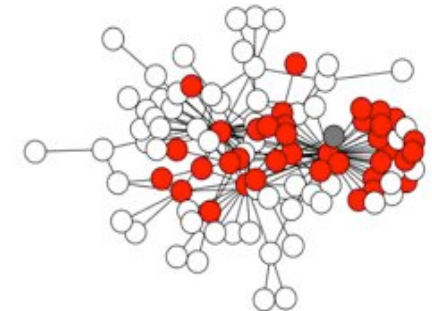
C. Castellano et al., "Statistical physics of social dynamics", Rev. Mod. Phys. 81, 591 (2009)

F. Colaiori et al., "A general three-state model with biased population replacement: analytical solution and application to language dynamics", Phys. Rev. E (to appear).

Spreading processes on complex networks

Dynamical processes have been studied for decades on regular lattices and their behavior is generally well understood. When such processes take place on a complex topology, what is the effect of the disordered interaction pattern on their phenomenology? In recent years I have been in particular involved in the investigation of the behavior of spreading processes, which range from infectious disease epidemics to "social contagion", i.e.,

information diffusion or meme propagation. Complex networks topology has a very strong impact on epidemic processes, facilitating spreading and increasing the risk of pandemics. Nontrivial effects are responsible for this vulnerability and their understanding challenges established theoretical approaches.



The study of epidemic-like spreading processes in the social domain, spurred by that the "big data" revolution is a very active and promising field for future research.

C. Castellano and R. Pastor-Satorras, "Threshold for epidemic spreading in networks", Phys. Rev. Lett. 105, 218701 (2010).

M. Boguna' et al., "Nature of the Epidemic Threshold for the Susceptible-Infected-Susceptible Dynamics in Networks", Phys. Rev. Lett. 111, 068701 (2013).

R. Pastor-Satorras, C. Castellano, P. Van Mieghem and A. Vespignani, "Epidemic spreading in networks", Rev. Mod. Phys. 87, 925 (2015).





Andrea Cavagna

Sapienza unit

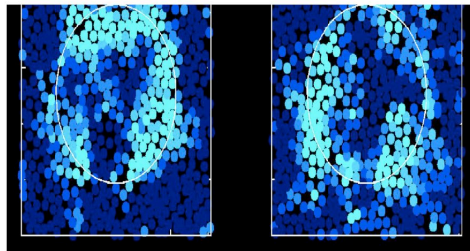
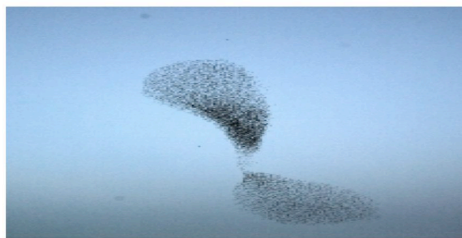


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keywords

- *Collective Behavior in Biological Systems*
- *(Non-Equilibrium) Statistical Mechanics*
- *Inference, Modeling & Simulations*



Collective Behavior in Biological Systems

The basis of our overall methodology is linking the experimental data (observed behaviour) with the theories explaining the interactions rules governing large animal groups. This broad mandate requires an interdisciplinary approach ranging from field experiments, to computer vision, to statistical physics. In general, we have split our focus in two areas: i) experimental data gathering and processing; ii) data analysis and theory. Our experimental work is carried out in the natural habitat of the animal we are studying. We use multiple synchronized high speed cameras to capture image sequences of the aggregation. By using novel computer vision algorithm, we are then able to reconstruct the 3D trajectories of each individual in the group. Our data analysis follows a theoretical approach inspired by the principles of statistical physics.

Many-body physics in real time

I am working on devising new methods to detect a growing static correlation length in deeply supercooled liquids. By using amorphous boundary conditions we measured for the first time a thermodynamic correlation length. In so doing we test the validity of different theoretical frameworks of the glass transition, namely the Adam-Gibbs theory and the Mosaic (aka Random First Order) theory. We are also trying to measure the surface tension between different amorphous phases in deeply supercooled liquids and to establish a link between static relaxation and dynamic heterogeneities through the concept of surface tension. Check my pedagogical reviews on spin-glasses and supercooled liquids, Spin-Glass Theory for Pedestrians [J. Stat. Mech. (2005) P05012] and Supercooled Liquids for Pedestrians, Physics Reports 476, (2009), P51



Stefano Selci

Tor Vergata unit



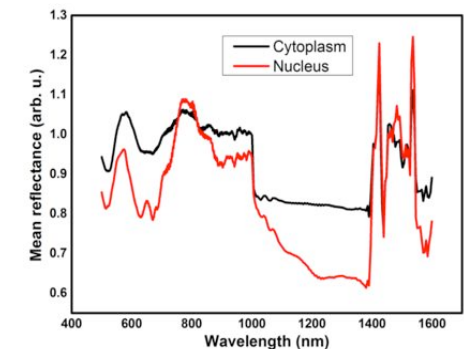
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keywords

- *Analisi morfologiche di cellule e tessuti mediante tecniche di microscopia ottica, confocale ed elettronica*
- *Analisi spettroscopica uv-vis-nir*
- *Microscopia a scansione di sonda*

Stefano Selci shows strong competences in experimental solid state physics, in particular optical spectroscopy and other surface techniques like scanning probe microscopies. Later involvements in some newer optical techniques or technological efforts, like instruments for space missions, in which nanotechnology competences acquired within the STM have been applied, display his great curiosity and ability to exploit competences in different disciplines. The combination of well proven skills in optical spectroscopy and scanning probe concepts has enabled Stefano Selci to build a new type of confocal microscope. The acquisition of images with high spatial resolution X,Y and Z, typical of any confocal microscope, has been combined with the hyperspectral acquisition of an extended and continuous spectrum from the visible to medium infrared regions.



Stefano Selci is author or co-author of about 100 papers published in national and international journals and books, several patents, and has supervised several theses for degrees and PhDs in Physics. He has also organized NATO schools and has been Editor of Conference books. He is a regular referee for international journals (e.g. Journal of Applied Physics). He has been Adviser for the Nobel Prize assignment in Physics (2002).



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keywords

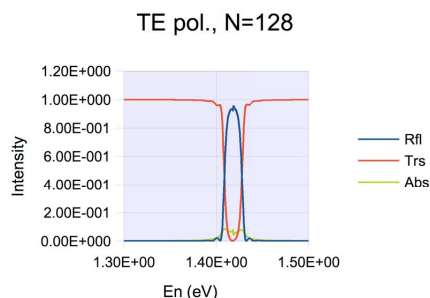
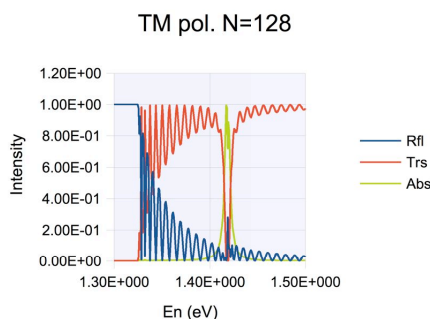
- Linear optical properties of isotropic-anisotropic etherostructures
- Exciton-polariton propagation in isotropic-anisotropic multilayers

Linear optical properties of isotropic-anisotropic etherostructures

The study intends to individuate the dynamical behavior of the light propagation in periodic etherostructures whose elementary cell is built alternating isotropic slabs with anisotropic ones with in plane optical axes mis-oriented among them. The resulting elementary cell shows spatial asymmetry that strongly affects the propagating modes of the system and their polarization state.

Linear optical properties of isotropic-anisotropic etherostructures

In this case the research focuses on systems showing a periodic mis-orientation of the in plane C_{axis} and an excitonic resonance in their isotropic part. As indicated by the optical response reported in the figures for a system of 128 unitary cells, $\delta\epsilon_c = \pi/2$, exciton energy $E_n = 1.418 \text{ (eV)}$ and for Bragg condition along x (TE direction)



the light-exciton interaction behaves as totally absorbing under TM radiation and as totally reflecting under TE, being always linear its polarization.



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keywords

- Transport of biopolymers in nanopores
- Statistical mechanics of complex systems
- Nonlinear Physics and Chaos

Transport of proteins

Nanopore technology is the "art" of retrieving chemical and physical information about biomolecules through their transport behavior across nanopores (nanoscale "holes") FigB. This field is considered the new frontier of single-molecule manipulation and sequencing with relevant applications to biology and medicine. Experiments are becoming very accurate and produce a countless number of facts and data which the theory is called to explain.

Main theoretical tools: Stochastic Processes, Modelling and Simulations, Statistical Mechanics.

Statistical mechanics of complex systems

Understanding complex phenomena like the emergence of collective or auto-organized dynamics in many-body systems requires to master advanced concepts and methods of statistical mechanics and stochastic process theory. Particular important is the modeling of complex systems which finds several applications e.g. to biology, material science, economic or social phenomena. We are interested to study complex behaviors in granular materials and transport processes.

Fig. Chain of nonlinear oscillators considered a paradigm of a complex system.

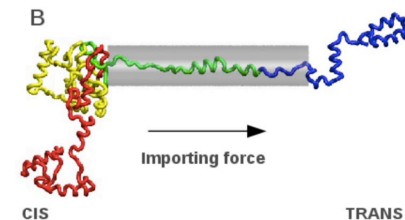
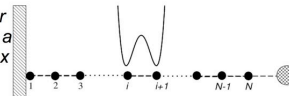
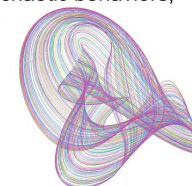


Fig. Transport of a protein by a pulling force

Nonlinear Physics and Chaos

Nonlinearity is a general element of natural phenomena and Chaos theory is the systematic study of the "unexpected" effects produced by nonlinearities. In particular, two initial conditions differing for an infinitesimal error, which according to Newton's physics would yield similar results, can lead to vastly different outcomes (Butterfly effect). The discovery that unpredictable behaviors are consistent with deterministic laws changed the way we perceive the world around us. Nonlinear physics is the interdisciplinary field that develops mathematical tools and concepts to classify and characterize: chaotic behaviors, strange attractors and the related fractal structures.

Fig. A strange attractor showing a fractal structure.





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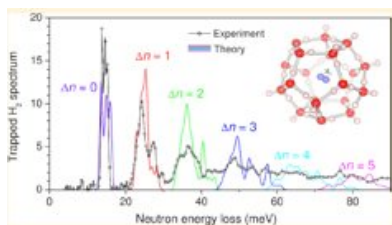
keywords

- Raman and neutron spectroscopy, neutron diffraction
- Confined hydrogen in nanostructured geometries
- Structure and dynamics in simple and quantum liquids
- Neutron instrumentation

Raman and inelastic neutron scattering on hydrogen clathrate hydrates

Clathrate hydrates are solid inclusion compounds, where water molecules constitute a regular lattice, characterized by the presence of polyhedral nano-cages, inside which guest molecules of a different compound are confined. The dynamics of the trapped molecules are well described in terms of localized excitations.

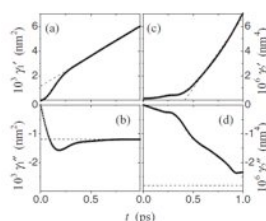
Considerable effort has been devoted in recent years to the study of hydrogen clathrate hydrates, because of their potential as efficient and environmentally friendly materials for hydrogen storage. In addition to this practical importance, hydrogen clathrates are also of considerable theoretical interest as prototypical examples of confined quantum particles.



M. Celli et al., J. Chem. Phys. **139**, 164507(2013)
D. Colognesi, J. Chem. Phys. **141**, 134501 (2014)

Non-Gaussian self-dynamics of liquid hydrogen

Understanding the single-particle, or self-dynamics of liquids is a longstanding research theme in condensed matter physics. One of the most important approaches to this problem is based on the so-called Gaussian approximation (GA), in which it is assumed that the motion of particles is only determined by the time autocorrelation function of the particle velocity (vaf). Although often adopted, the validity of GA is not yet well assessed in different wave vector ranges, especially for quantum Boltzmann liquids (i.e. H₂, D₂, Ne...). By mean of neutron spectroscopy investigation and quantum simulation we study the limits of the GA in the self dynamics of quantum liquids and we determinate the first non-Gaussian correction term.



M. Celli et al. Phys. Rev. B **84**, 140510(R), (2011)
D. Colognesi et al., Chem. Phys. **446**, 57 (2015)



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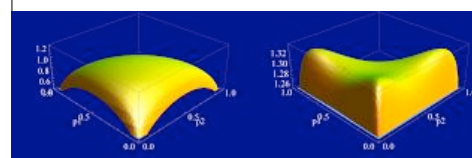
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keywords

- Non-Extensive entropy, power-law distributions
- Information geometry
- Nonlinear Fokker-Planck equations

Non-Extensive entropy

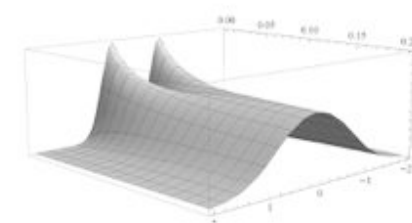


A wide variety of generalized entropies, from which probability distributions with power-law tails can be derived, are investigated on the epistemological point of view. Potential applications on physical and physical-like systems are considered.

Information geometry

Information geometry is a powerful framework for studying the family of probability distributions by applying the geometric tools developed in affine differential geometry. We apply this formalism to investigate the mathematical structure underlying non-extensive statistical mechanics.

Non-linear Fokker-Planck equations



Irreversible processes described by Fokker-Planck equations can be characterized by non-increasing Lyapunov functional. In non-linear FPEs Lyapunov functionals are related with generalized relative entropies.

publications

- Information geometry on the k-thermostatistics
Entropy 17, 1204
- Basic-deformed thermostatistics
J. Phys. A: Math. Theo. 40, 8635
- Entropic forms and related algebras
Entropy 15, 624



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keywords

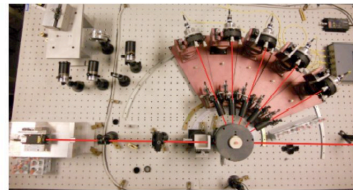
- Experiments of soft matter systems.
- Phase diagram. Gel and glass transitions.
- Structure and dynamics of colloids, polymers and bio-soft systems.

Structure and dynamics, phase diagram and gel/glass transitions.

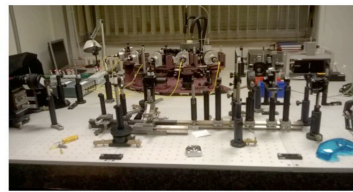
Structure and dynamics are investigated through conventional, synchrotron and neutron techniques. Measurements are performed, in collaboration with Dr. R. Angelini (ISC Sapienza), in the Soft Matter Laboratory: Light Scattering, in the Fermi Building room 010, where Dynamic Light Scattering (DLS), Multiangle DLS and Multispeckle DLS techniques are available (see Figures) and in Large Scale Facilities such as ESRF and ISIS.

Results are compared with theory and simulation in collaboration with Dr. E. Zaccarelli (ISC Sapienza).

In particular we investigate system different from common "hard" spheres colloidal ones such as:



Multiangle DLS

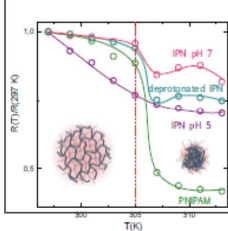


Multispeckle DLS

Anisotropic colloidal particles.

Charged colloidal suspension of disks of nanometric size with inhomogeneous charge distribution interacting through a directional "patchy like" potential. The phase diagram has been deeply studied offering also the possibility to observe unconventional arrested states.

Nature Materials **5**, 4049 (2014); *Nature Communications* **10**, 56 (2011).



Polymeric multiresponsive microgels

Microgels, made by interpenetrated polymer networks, thermo- and pH responsive. Highly used for technological applications and example of "soft" colloids partially interpenetrating that are expected to originate even more complex and fascinating phase diagrams respect to conventional colloids.

JNCS **407**, 361 (2015); *JCP in press* (2016).



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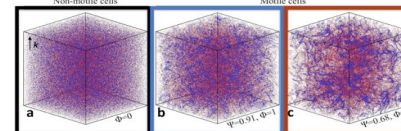
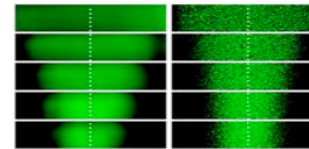
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keywords

- Turbulence and transport of fields and particles in turbulent flows
- Chaos and dynamical systems
- Population dynamics

Transport of swimming micro-organisms in turbulence

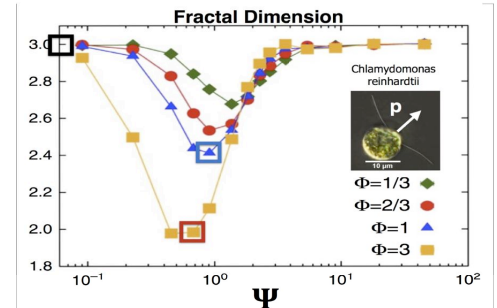
Substances transported by a turbulent flow typically mix quickly (e.g stirring milk into coffee). What does happen to **micro-organisms transported by a turbulent flow**? They are typically very small and have the same density of the fluid so that are expected to follow the fluid elements and thus to mix very efficiently. However, **if they can swim**, as bacteria or some species of algae, something **counterintuitive** can happen: **they can unmix forming fractal clusters**. This phenomenon has been studied experimentally, in a vortical flow, and numerically, in a turbulent flow, for gyrotactic microalgae.



W. M. Durham, E. Climent, M. Barry, F. De Lillo, G. Boffetta, M. Cencini, R. Stocker *Nature Comm.* **4**, 2148 (2013)

F. De Lillo, M. Cencini, W. M. Durham, M. Barry, R. Stocker, E. Climent, G. Boffetta, *Phys. Rev. Lett.* **112**, 044502 (2014)

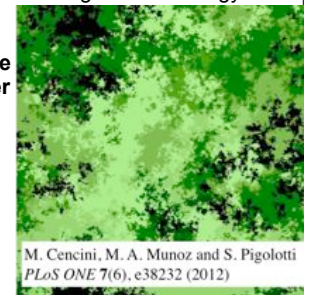
M. Cencini, M. Franchino, F. Santamaría, G. Boffetta, preprint arXiv:1511.01255 (2015)



Neutral biodiversity models

Species abundance distributions and how the number of species changes with the area (**Species Area Relationships**) can be captured by simple neutral models, with a flat "fitness" landscape. Efficient algorithms have been developed to study nontrivial regimes of small speciation rate and large local population sizes, relevant to microorganisms ecology. We found

that **large local populations give rise to shallower SAR, in accord with field observations.**



M. Cencini, M. A. Munoz and S. Pigolotti *PLoS ONE* **7**(6), e38232 (2012)



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keywords

- Network Science
- Quantitative Linguistics
- Biophysics

Interdisciplinary research
Physics as a tool

typical problems

Structure of Social Networks

Social networks have empirically been found to be *assortative* (i.e., the degrees of neighboring nodes are positively correlated), while other networks (e.g., technological, biological) show the opposite pattern (*disassortative*). Why is that so?

How do these patterns change in *signed networks*, where relations indicate trust/distrust, friendship/enmity? Do individuals who dislike many others tend to dislike each other, or do they dislike those who dislike only very few others?



Rules and Exceptions in Language Dynamics

In all languages, rules have exceptions in the form of irregularities. Since rules make a language efficient, the persistence of irregularity is an anomaly. How do language systems become rule governed? How and why do they sustain exceptions to rules? Frequent words are unlikely to change over time (e.g., frequent verbs tend to maintain an irregular past tense form). What is the role of frequency in maintaining exceptions to rules?

Dynamics of Virus-Host interaction

In the case of fast mutating viruses (e.g., Influenza virus), the virus-host interaction is driven by *cross-immunity*: after being infected by a strain, the host acquires immunity to a set of other strains *antigenically similar* to the infecting one (i.e., triggering the same host immune response). The evolutionary dynamics of viruses is then ruled by their relative *antigenic distance*. Can we understand the nontrivial relation between antigenic and genetic distance?



methods

Tools from statistical physics, modeling, analytical approach (whenever possible), simulations, data analysis, web-based experiments.



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keywords

- Mathematics
- Tunneling
- Complexity in society, and economics

Macroscopic quantum tunneling

The principle that no signal can travel faster than the light speed in vacuum is accepted as one of the basic laws of nature. Yet, there is no formal proof, based only on Maxwell's equations, that no electromagnetic wave packet can travel faster than the speed of light.

Therefore, there may be a shadow of doubt as to whether this principle is true in any case. However, the question as to whether a wave packet can be considered a signal is a much debated and complicated one. Superluminal effects for evanescent waves have been demonstrated in tunneling experiments in both the optical domain and the microwave range.

Complex systems and economic crises.

Economic theory dominant today, known as the neoclassical synthesis, assumes that markets are in equilibrium as demand always equals supply.

The financial crisis which started in early 2007 and still not resolved yet, has shown that the economic and financial system, far from being in a state of equilibrium, is, manifestly, in a constant state of instability.

The science of complexity is proving to play an important role in the modeling of economic events and social phenomena as systems that evolve in the non-equilibrium.

Our goal is to achieve better understanding of the issues outlined above.



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keywords

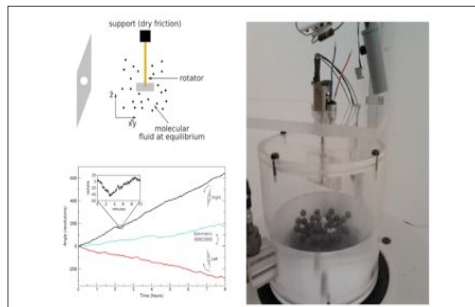
- Granular materials
- Out-of-equilibrium statistical physics
- Brownian motors

Granular materials

Granular media are systems made of many “grains” (particles from 0.1mm or larger) which lose energy when interacting. They are a fascinating testground for many recent theories in out-of-equilibrium statistical physics (see below). Here we study those systems by numerical simulations, kinetic theories and experiments. You can have a look to our lab at the ground floor of Fermi Building, Room 012.

Out-of-equilibrium statistical physics

Equilibrium statistical physics fails in many systems where currents and dissipation appear (turbulence, forced fluidodynamics, aggregate of self-propelled particles, open systems, etc.). Many alternative approaches exist, such as hydrodynamics and kinetic theory, e.g. the Boltzmann equation.



Sometimes these systems are also “small” and for this reason fluctuations can be very large: the theories of probability, stochastic processes, and large deviations, become – therefore - essential tools.

Brownian motors

They are small objects that “rectifies” fluctuations, obtaining work from heat. We study models and experimental examples, showing in which (non-equilibrium) conditions such a rectification may be optimized.



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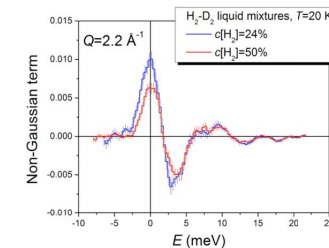
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keywords

- Inelastic Neutron Scattering
- Hydrogen and Hydrogen-containing Materials
- Dynamics of Quantum and Semi-quantum Fluids
- Neutron Scattering Instrumentation

Inelastic Neutron Scattering on a Composite of NaAlH₄ and Nanoporous Carbon

Inelastic neutron scattering spectra of a melt-infiltrated composite of NaAlH₄ and active carbon fibers have been studied at low temperature for two sample conditions: as prepared and subjected to hydrogen desorption-absorption cycling. After a careful data analysis, the experimental results have been compared to the corresponding spectroscopic data taken from bulk NaAlH₄ and Na₃AlH₆. Evident signatures induced by infiltration process onto the NaAlH₄ phonon bands have been detected, showing up as a strong peak broadening and smoothing together with, in some cases, an energy shift. Traces of Na₃AlH₆, appearing as an extra intensity between 130 and 200 meV, seem also confirmed. Further work, both experimental and based on *ab initio* simulations, is surely needed in order to rationalize the finding of the present measurements.
D. Colognesi *et al.*, *J. Phys. Chem. A* **115**, 7503 (2011).
D. Colognesi *et al.*, *J. Phys. Chem. A* **117**, 7314 (2013).



Non-Gaussian effects in the self dynamics of semi-quantum fluids

An extension of the non-Gaussian correction to quantum fluids is devised, with a particular interest in the so-called semi-quantum liquids. In this case a detailed correction scheme for both the short- and the long-time behaviors of the intermediate scattering function is proposed. Subsequently, a practical test of this approach is performed on neutron scattering spectra derived from liquid para-H₂ and para-H₂ plus normal D₂ mixtures. These experimental findings confirm the validity of our approach and show that a description of the self dynamics beyond the Gaussian approximation is necessary even in simple liquids affected by mild quantum effects.
D. Colognesi *et al.*, *Chem. Phys.* **446**, 57 (2015).





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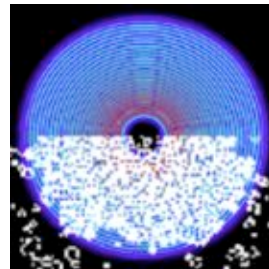
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keywords

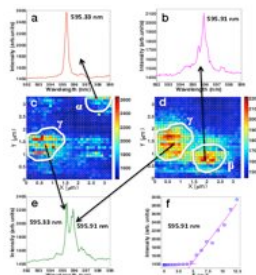
- *Photonics and nonlinear optics, experiments and theory*
- *High performance computing*
- *Theoretical physics*

The enlightened game of life

Is complexity linked with light? We decide if something is complex or not by observing its structure and hence interacting with electromagnetic waves. Is this fact more fundamental than that? We want to develop theoretical models for assessing the link between light and complexity, starting from the simplest one: the Conway's Game of Life



Random lasers, experimental activity



Complexity arises when there is disorder and nonlinearity. Photonics is full of examples in which highly nonlinear regimes occur in the presence of disorder. The case of light-matter interaction in random systems is specifically important for a novel class of devices named random lasers. In our laboratory we study random lasers in bio-templated materials and other complex systems.

Quantum gravity simulation

Highly nonlinear regimes in optics are formally identically to quantum gravity enhanced quantum mechanics, including a generalized uncertainty principle. Can we simulate quantum gravity in the lab?

$$\Delta X \Delta P \geq \frac{\hbar}{2} (1 + \beta \Delta P^2)$$



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keywords

- *Nonlinear Optics*
- *Numerical Simulations*
- *Lasers*

Stochastic Simulator for modeling the transition to lasing

With G.L.Lippi

A Stochastic Simulator (SS) is proposed, based on a semiclassical description of the radiation-matter interaction, to obtain an efficient description of the lasing transition for devices ranging from the nanolaser to the traditional "macroscopic" laser. Steady-state predictions obtained with the SS agree both with more traditional laser modeling and with the description of phase transitions in small-sized systems, and provide additional information on fluctuations. Dynamical information can easily be obtained, with good computing time efficiency, which convincingly highlights the role of fluctuations at threshold.

Slow dynamics in semiconductor multi-longitudinal-mode laser transients governed by a master mode

With G.L.Lippi

We examine the response to the sudden switch of the pump parameter in a multimode semiconductor laser with intensity coupling on a model whose validity has been successfully compared to experimental results. We find the existence of a very slow modal evolution governed by a master mode, which reaches its steady state on a time scale that is a couple of orders of magnitude longer than that of the total intensity.

Fast dynamics and spectral properties of a multilongitudinal-mode semiconductor laser: evolution of an ensemble of driven, globally coupled nonlinear modes.

With G.L.Lippi

We analyze the fast transient dynamics of a multi-longitudinal mode semiconductor laser on the basis of a model with intensity coupling. The dynamics, coupled to the constraints of the system and the below-threshold initial conditions, imposes a faster growth of the side modes in the initial stages of the transient, thereby leading the laser through a sequence of states where the modal intensity distribution dramatically differs from the asymptotic one. A detailed analysis of the below-threshold, deterministic dynamical evolution allows us to explain the modal dynamics in the strongly coupled regime where the total intensity peak and relaxation oscillations take place, thus providing an explanation for the modal dynamics observed in the slow, hidden evolution towards the asymptotic state





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keywords

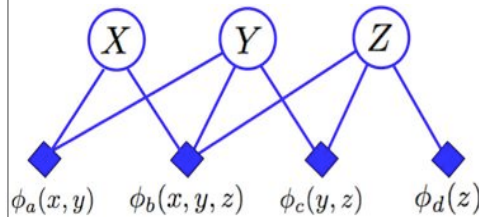
- Complex fluids
- Statistical inference and combinatorial optimization
- Random graphs

Thermodynamic anomalies of water

Water is an ubiquitous substance, which nonetheless exhibits an impressive amount of anomalous properties, among which the well known density maximum at 4°C at atmospheric pressure. Simple statistical-mechanical models can qualitatively describe such anomalies, and may help investigate the conjectured connections with supercooled and glassy states of water.

Random graph theory

The cavity method is an advanced mean-field technique, generally used to study disordered systems. This method can also be employed to investigate some issues in *random graph theory*, for instance the emergence of extensive regular subgraphs.



Graphical model of a generic statistical-inference problem

Belief Propagation

A lot of *statistical-inference problems* of high technological importance (for instance: error-correction for digital transmission over a noisy channel) can be formalized in terms of calculation of a Boltzmann distribution for Ising- or Potts-like models defined on heterogeneous graphs. Belief Propagation is a very efficient algorithm to perform such calculations, based on a statistical-mechanical method of the mean field type (Bethe-Peierls approximation).



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keywords

- dynamics of point defects and domain walls, phase transitions
- ferroelectric, magnetic, superconducting, ion conducting perovskites
- dynamic elastic properties of solids

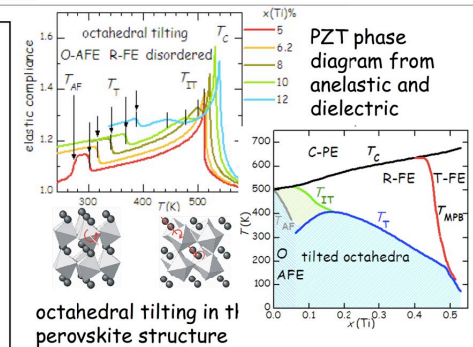
Phase diagrams of ferroelectric perovskites

The dynamic elastic properties of ferroelectric (FE) perovskites are studied in close collaboration with Floriana Craciun for the dielectric properties.

$\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$ (PZT) has been studying for 60 years and is the most used piezo-electric material, but the newly measured elastic compliance, with anomalies in correspondence of all the structural transitions, entails a revision of the phase diagram, e.g. with new tilt instabilities of the ZrO_6 octahedra and splitting of the polar and tilt modes at the antiferroelectric transition. These new features are under study by other techniques through international collaborations.

The need to obtain materials with properties similar to PZT or improved but without the toxic Pb has boosted the study of the mechanisms enhancing the piezo-electric activity of PZT and similar materials at the morphotropic phase boundary (MPB) between FE rhombohedral and tetragonal phases. A maximum in the compliance in correspondence with the MPB of PZT and the Pb-free materials NBT-BT and BCT-BZT has been shown to be due to the intrinsic ability of the polari-zation to easily rotate, rather than only an extrinsic effect from domain wall motion.

F: Cordero *et al.* Phys. Rev. Lett. **98**, 255701 (2007).
F: Cordero *et al.* Phys. Rev. B **81**, 144124 (2010).
F: Cordero *et al.* Appl. Phys. Lett. **103**, 122903 (2014).



octahedral tilting in tl perovskite structure

Defects, ion conduction and polarons

The anelastic spectra vs T at different frequencies allow the relaxation, hopping and reorientation frequencies of point and extended defects and polarons to be measured.

In particular, O vacancies are difficult to study with other techniques, though they heavily affect the materials properties as unwanted defects, ionic charge carriers or dopants. Our studies are focused on H and O vacancies in SrTiO_3 , ferroelectric, super- and ion conducting perovskites.

We also study the metal-insulator and magnetic transitions involving Jahn-Teller distortions in manganites and nichelates.

F: Cordero, Phys. Rev. B **76**, 172106 (2007).
F: Cordero *et al.* Phys. Rev. B **82**, 104102 (2010).
F: Cordero *et al.* Phys. Rev. B **84**, 125127 (2011).



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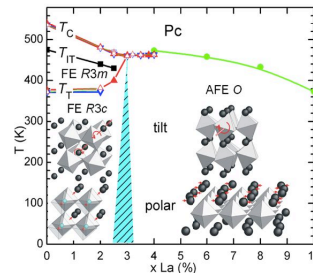


- Phase transitions
- Nanostructured polar materials
- Multiferroic materials

Phase diagrams of antiferroelectric and ferroelectric perovskites

The dielectric properties of these materials are studied in close collaboration with Francesco Cordero for the anelastic properties. Recent results allowed to refine the phase diagram of La-doped $\text{PbZr}_{0.9}\text{Ti}_{0.1}\text{O}_3$, interesting for electro-optical applications, high energy density capacitors, digital displacement transducers etc., near the phase boundary between competing antiferroelectric and ferroelectric phases.

F. Craciun *et al.*, J. Appl. Phys. **117**, 184103 (2015).

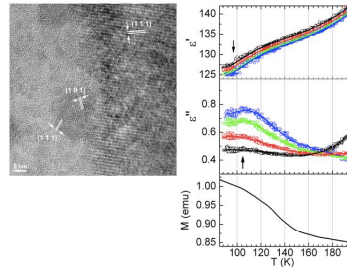


Multiferroicity of ferroelectric perovskites doped with magnetic impurities

Multiferroic materials that exhibit simultaneously magnetic and ferroelectric (FE) order are investigated due to their potential applications in multifunctional sensors, spintronics, data storage, etc. We found emergent magnetic properties in (Sm,Fe)-doped PbTiO_3 FE perovskite and an abnormal behavior of dielectric constant and loss below the temperature where the magnetization also increases. HRTEM evidenced a polar nanostructure, besides normal FE domains.

F. Craciun *et al.*, Appl. Phys. Lett. **102**, 242903 (2013).

F. Craciun *et al.*, J. Appl. Phys. **116**, 074101 (2014).



Nano/macro domain transitions in nanostructured polar materials

We have investigated thermally driven and electrically driven nano/macro domain transformations in different nanostructured polar materials like NBT-BT and PLZT. Such transformation has been evidenced also in epitaxial PLZT thin films under anisotropic strain.

F. Craciun *et al.*, Appl. Phys. Lett. **102**, 162902 (2013).

F. Craciun *et al.*, J. Appl. Phys. **112**, 124106 (2012); N. Scarisoreanu *et al.*, J. Appl. Phys. **116**, 074106 (2014);

F. Craciun, Phys. Rev. B **81**, 184111 (2010).



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keywords

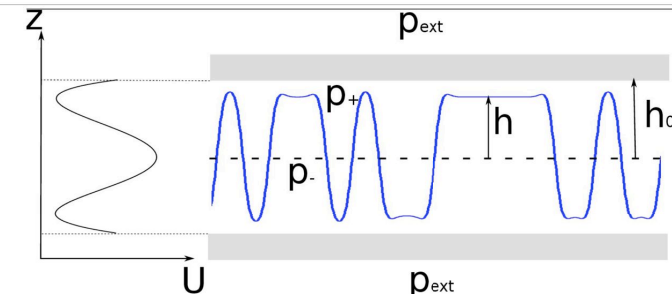
- Nonequilibrium statistical physics
- Nonlinear dynamics
- Pattern formation

Dynamics and energetics in far from equilibrium systems

A physical system which is relaxing towards equilibrium and a system *driven* far from equilibrium may display some common features: the instability of an homogeneous state, the rising of a new structured state and the adjustment of its typical length scale. These phenomena can be observed in biophysics, condensed matter, atomic physics, granular materials, and so on. Relevant questions are: What are the dynamics of the system? Do they depend on energetic factors? Is the system able to attain the ground state and on what time scale?

For example, in some cases dynamics can be frozen. This is the case for the biological membrane depicted in the figure below and confined between walls, where the membrane adheres to both walls. The resulting structure of adhesion patches is ordered or disordered depending on wall permeability and it is frozen because the energy of the membrane depends on its curvature (via bending rigidity) rather than by its total length (through surface tension). If surface tension or fluctuations are substantial, they may trigger a coarsening process where the size of adhesion patches increase in time.

The figure illustrates the main ingredients: the adhesion potential (left) and the effect of bending rigidity, which induces oscillations in the patches attached to the walls.



In collaboration with Thomas Le Goff and Olivier Pierre-Louis (Lyon).



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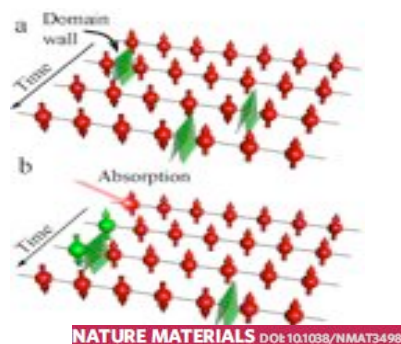
keywords

- Magnetism in low-dimensional systems
- Molecular magnetic chains
- Ultrathin magnetic films

Dynamic control of magnetic nanowires by light-induced domain-wall kickoffs

(a) The time evolution of the paradigmatic Ising magnetic molecular nanowire $\text{Co}(\text{hfac})_2\text{NITPhOMe}$ is normally described by Glauber dynamics, consisting in domain-wall nucleation (with energy cost $2J$, where $J \sim 75$ K is the intrachain exchange constant) and subsequent propagation via a random-walk process (at no energy cost). The resulting relaxation time of the magnetization follows an Arrhenius law, $\tau = \tau_0 \exp(2J/T)$, where the spin-flip attempt rate is $\tau_0 \approx 4 \times 10^{-11}$ s.

(b) By continuous irradiation of the sample by a HeNe laser ($\lambda = 632.8$ nm) at low power ($\approx 1 \mu\text{W}/\text{cm}^2$), a much faster decay of the magnetization, $\tau_{\text{exc}} = \tau_0 \exp(2J_{\text{exc}}/T) \gg \tau$, is obtained. This is realized through a kickoff mechanism. The adsorption of a photon at one site of the chain creates a Frenkel exciton. For the exciton duration, $\tau_{0,\text{exc}} \approx 10^{-8}$ s $\gg \tau_0$, the intrachain exchange coupling with a spin at the exciton site (green arrow) becomes $J_{\text{exc}} \approx 50 \text{ K} < J$. The above mechanism is perfectly reversible, proving that Glauber's stochastic dynamics of the Ising model can be easily controlled using light with power nearly 1000 times smaller than in previous optical switching methods.



Rotatable magnetic anisotropy in FeGa films with stripe domains

In magnetoelastic films of FeGa, the spontaneous formation of an up/down stripe domain structure is induced (for film thickness greater than a critical value $t_c \approx 40$ nm) by the competition between the easy-plane magnetic dipolar interaction and a moderate perpendicular magnetic anisotropy. Using Brillouin light scattering to study the spin-wave excitations in a 65 nm $\text{Fe}_{0.8}\text{Ga}_{0.2}$ film (PRB **89**, 024411), we have shown that the stripe pattern is associated with a nonzero "rotatable" magnetic anisotropy (effective field $H_{\text{rot}} \approx 1 \text{ kOe}$), so named because the stripes orientation in the film plane is determined only by the sample history (direction of the last saturating field).



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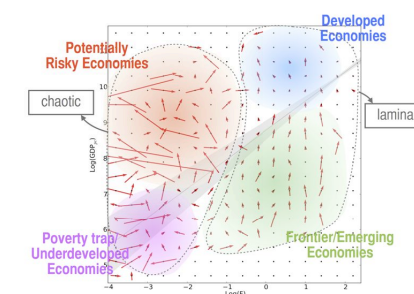
keywords

- Economic Complexity
- Finance
- Agent-Based Modeling & Self-Organization of Markets

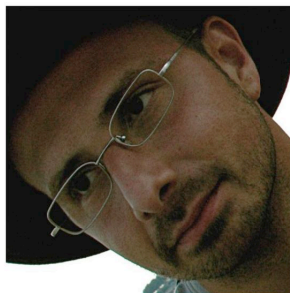
Economy can be portrayed as a complex adaptive process and competitiveness cannot be seen anymore as the final result of equilibrium systems where feedbacks are linear and uncoupled. The present data-centric era, methods from complexity and dynamical systems provide a unique opportunity to lead the scientific shift of the economic thinking and ground it empirically.

The heterogeneous dynamics of Economic Complexity: what will be the growth of the GDP and the competitiveness of China, the USA, Vietnam and Sierra Leone in the next 10 years? The answer is 'it depends': predicting the evolution of fitness and income is strongly dependent on the regime a country occupies. There exist economic regimes for which the fitness (a synthetic measure of the country competitiveness) is able to effectively uncover the hidden potential of growth of countries. Forecasting country growth faces hurdles which are similar those found in predicting dynamical systems (i.e., the atmosphere, climate, wind and ocean dynamics). On this account there is strong evidence for a high degree of heterogeneity in the growth dynamics of countries. We observe the emergence of different regimes of economic complexity and in particular there are several regimes for the patterns of evolution of

countries in the fitness-income plane, as illustrated in the figure. Depending on the position in the fitness-income plane, we are able to distinguish two main regimes: a laminar-like regime in which the fitness appears to be predictive, or at least informative, of country growth; and a chaotic regime in which the fitness is poorly or completely uncorrelated with the evolution of the wealth of those countries.



Tacchella et al. Scientific Reports **2**, 723 (2012).
Cristelli et al. PloS ONE **10**(2):e0117174 (2015).



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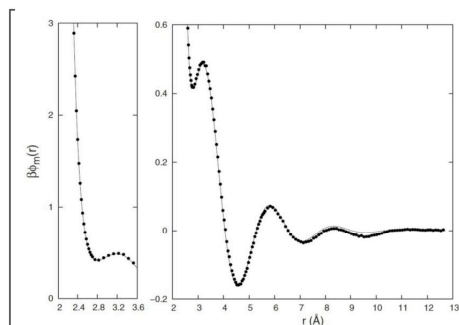
keywords

*Statistical mechanics and Monte Carlo methods
Optical microscopy and spectroscopy
Instrument development for space*

Monte Carlo solution of the inverse problems in classical statistical mechanics

Analysis of the “inverse-problem” for classical statistical systems, both in the continuum and on the lattice. I have developed a procedure, based on the application of the Maximum Entropy Principle, for the determination of the microscopic interaction potential starting from the knowledge of a set of correlation functions.

M. D'Alessandro and F. Cillico, *Physical Review E* **82**, 021128 (2010) [arXiv:1006.3656]
M. D'Alessandro, *Physical Review E* **84**, 041130 (2011) [arXiv:1206.4811v1].



Reconstruction of the interaction potential of a model of liquid Aluminum at high density

Development of scientific instrument for space-type applications

Development and realization of a shutter for neutral atoms for the ELENA instrument, as part of the ESA mission “BepiColombo”.

Hyperspectral confocal microscopy

Theoretical analysis of light interaction with multi layered systems in confocal microscopy



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keywords

- *Exciton-polaritons*
- *Photonic-crystals*
- *Microcavities*

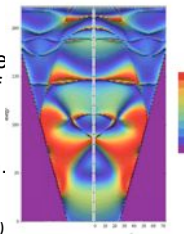
Microcavity polaritons

The composite boson nature of excitons plays a key role in their many-body physics. The undistinguishability of the two carriers leads to different exchange processes that enter ex-ex interactions and are a source of nonlinearity in the optical properties of semiconductors. A composite boson formalism is then necessary to study polariton-polariton scattering in semiconductor microcavities.

L. Piloizzi et al. *Phys. Rev. B* **82**, 075327 (2010)
M.M.Glazov et al. *Phys. Rev. B* **80**, 155306 (2009)

Subwavelength gratings

Artificial electromagnetic media, achieved by structuring on the subwavelength scale, are an important tool in modern optics to enhance device performance by engineering the electromagnetic space and controlling waves propagation. Structured surfaces, as free standing dielectric gratings, can be designed to act as mirrors since they show scalable energy bands of high reflectivity, polarization sensitive. Placed in a cavity volume they allow the tailoring of the electric field intensity and the enhancement of light-matter interaction.



L. Piloizzi et al.
Phys. Rev. B **86**, 045301 (2012)

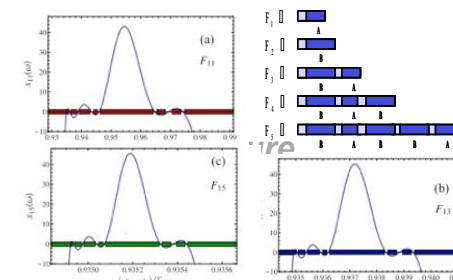


Fig.1) Trace scaling for a Fibonacci resonant structure.

Resonant photonic crystals

Are sequences of sites with resonant excitations long range coupled through an electromagnetic field. They can form wide energy band gaps, as in periodic photonic crystals, and localized states as in disordered media.

Fibonacci and Thue-Morse chains demonstrate scaling invariance and self-similarity for exciton-polariton dispersion. (Fig.1).

Bichromatic structures with compound non-centrosymmetric unit cells, following the off-diagonal Harper model, show topological properties as the existence of protected edge states.

A. N. Poddubny, et al. *Phys. Rev. B* **80**, 115314 (2009)
A. V. Poshakinskiy, et al. *Phys. Rev. Lett.* **112**, 107403 (2014)



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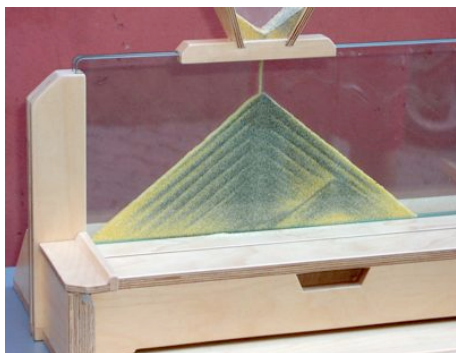
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keywords

- Dynamics of granular matter
- Disordered materials
- Complexity in society, biology and economics

Topic 1

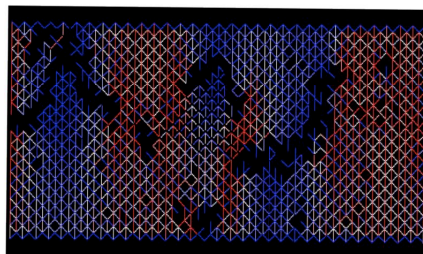
In our world, granular matter is more ubiquitous than crystals, however its dynamics is much less understood. Grains also provide a laboratory model for earthquakes and dissipative processes. We try to improve our understanding of the collective dynamics of grains performing laboratory experiments and numerical simulations, and try to describe it by means of stochastic processes.



Topic 2

Structural phenomena occurring in disordered materials often bring the features of criticality, i.e. long range correlations and self similar patterns, like for example in the pattern of a propagating

crack. Despite their complexity, it is often possible to understand and describe these phenomena by means of simple models like cellular automata and lattice gas.



Topic 3

Understanding the dynamics underlying human and biological activities is difficult. However the now available large amount of data provides lot of information. We are presently investigating the mutual import-export relations of world-wide countries, pointing out analogies with some ecological systems.



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keywords

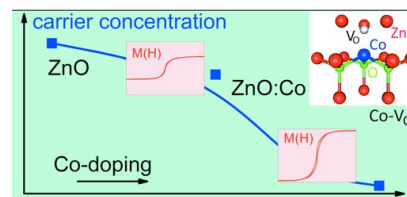
- Doping, defects and ferromagnetism in oxide-based materials
- Laser growth and processing of thin films and nanostructures

• Dilute magnetic oxides

Dilute Magnetic Oxides exhibit room temperature ferromagnetism whose origin is still unclear in most cases.

In $Zn_{1-x}Co_xO$ the occurrence of ferromagnetism can be associated to the concurrent presence of defects formed by oxygen vacancies close to Co atoms (Co-Vo complexes) and charge carriers. A qualitative picture explains the long-range ferromagnetic coupling of the Co atoms involved in the Co-Vo complexes.

We also investigate the effects of hydrogen irradiation on ferromagnetism and carriers of $Zn_{1-x}Co_xO$ samples.



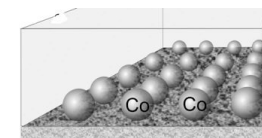
Effect of Co doping on conductivity and ferromagnetism in $Zn_{1-x}Co_xO$ thin films.

Ref. J. Mater. Chem. C 3, 10188 (2015)

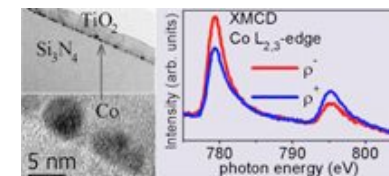
• Pulsed Laser Deposition of thin films and nanocomposites

The growth of thin films of nanocomposite materials by pulsed laser deposition indicated a route to synthesize metallic nanocrystals with well-defined position in a semiconducting matrix.

By proper selecting process parameters and materials it is possible to assemble on demand composite multifunctional materials at the nanoscale for reliable magneto-optical and plasmonic applications.



Planar arrays of Co nanocrystals in polycrystalline TiO_2 .



Ref. J. Phys. Chem. C 117, 687, (2013)





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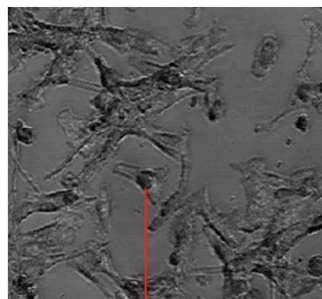
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keywords

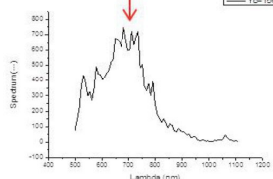
- *Hyperspectral Imaging*
- *Electronic properties of surfaces and interfaces*
- *ARPES from self-assembled systems of reduced dimensionality*

Confocal MicroSpectroscopy on biological systems in vitro and in vivo

The application of the hyperspectral confocal reflectance microscope led to the definition of a non-invasive and label-free method for discrimination of cells in co-culture. It is currently directed to the study of living cells and tissues with the aim of looking for the correlation between optical data and the formation of carcinomas and specific genetic defects of the skin.

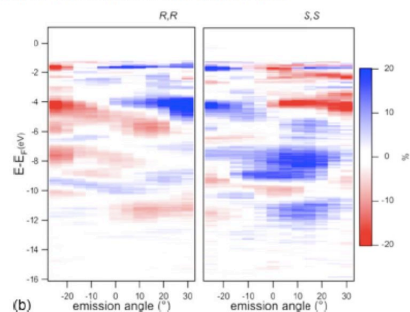


Melanocyte cell image and its spatially resolved reflectivity



Physics of low-dimensional materials

The study of the electronic properties of nanostructured systems with different geometry is of fundamental importance for the development of new nanostructured functional materials. We are interested in exploring : the effects of finite size and interface on the electronic and magnetic properties of ultra-thin films and multilayers; the high resolution (energy and momentum) electronic structure of magnetic and non-magnetic material with large spin-orbit interaction; graphene grown on metal substrates; self-organized chiral molecules on surfaces.



Maps of the dichroic signal for two enantiomers of *chiral molecules*, acquired by angular resolved photoemission with circularly polarized light
Ferrari L. e al. Phys.Rev. B 91, 085408 (2015)



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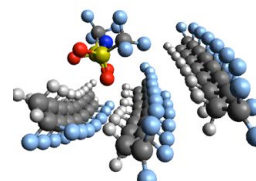
keywords

- *Spectroscopies*
- *Innovative materials for energy storage*
- *Phase transitions*

Ionic liquids and their interactions with membranes

Ionic liquids (ILs), which are inorganic salts with melting point below 100°C are environmentally friendly solvents with useful properties. Moreover their attractive properties can be tuned by variation of the cation and anion. Our research is focused to achieve a better physical understanding of the ions interactions and dynamics within the liquids by means of infrared and mechanical spectroscopies, thermal analysis and ab initio simulation.

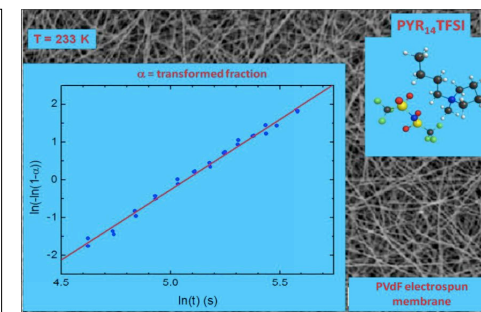
The occurrence of phase transitions and their kinetics is studied too. In particular, it is showed that in the composite systems usually used for applications, the interaction with the swelling membrane modifies the physical properties of ILs.



F. M. Vitucci, J. Manzi, M. A. Navarra, O. Palumbo, F. Treguadrini, S. Panero, P. Bruni, F. Croce, A. Paolone, J. Phys. Chem. C **118** 5749-5755 (2014).

F. M. Vitucci, F. Treguadrini, O. Palumbo, J.-B. Brubach, P. Roy, A. Paolone, J. Phys. Chem. A **118** 8758-8764 (2014).

F. M. Vitucci, O. Palumbo, F. Treguadrini, J.-B. Brubach, P. Roy, F. Croce, A. Paolone, J. Phys. Chem. C under review.



New materials for lithium batteries

We investigate the fundamental properties of new materials considered as promising as high energy density electrodes for lithium batteries, such as $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO) or LiCoPO_4 (LCPO). We studied the disorder of LNMO by means of EXAFS, the vacancy dynamics in LNMO by anelastic spectroscopy and the infrared phonon spectrum of LCPO.

G. Greco, S. Brutti, F. M. Vitucci, L. Lombardo, M. Koentje, A. Savoini, A. Paolone, S. Panero, J. Phys. Chem. C doi:10.1021/jp5063622.

F. M. Vitucci, O. Palumbo, A. Paolone, R. Cantelli, S. Brutti, S. Panero, J. Alloys Compds. **604** 83-86 (2014).

S. Brutti, J. Manzi, D. Di Lecce, F. Vitucci, A. Paolone, F. Treguadrini, S. Panero, Mat. Lett. under review.



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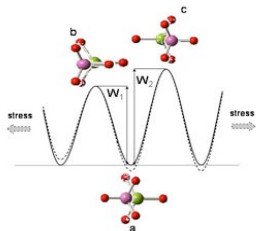
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keywords

- Spectroscopies
- Innovative materials for energy storage
- Phase transitions

Materials for hydrogen storage

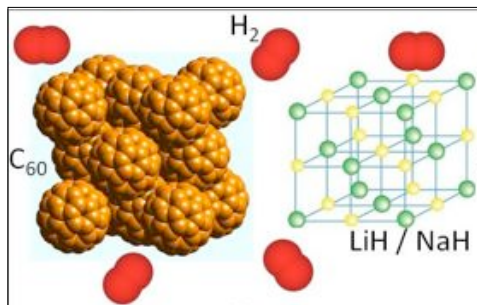
The most promising way to store hydrogen is the solid state storage, but at present a lot of fundamental research is still needed to make such solid state tanks satisfactorily compatible with the targets of current applications. Best candidates are metal hydrides and complex hydrides. A big role in increasing their capacity and enhancing the hydriding and dehydriding kinetics is played by the artificial manipulation, like nanostructuring of the powders, their mechanical alloying and catalysing. We study the hydrogenation and dehydrogenation fundamental mechanisms of such novel materials by means of mechanical and infrared spectroscopies, thermal analysis and ab initio simulation.



A. Paolone, F. Teocoli, S. Sanna, O. Palumbo and T. Autrey, J. Phys. Chem. C **117** 129-134 (2013).

A. Paolone, F. Vico, F. Teocoli, S. Sanna, O. Palumbo, R. Cantelli, D.A. Knight, J. Trepovich and R. Zidan, J. Phys. Chem. C **116** 16365-16370 (2012).

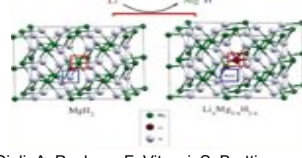
A. Paolone, O. Palumbo, P. Rispoli, R. Cantelli, T. Autrey, A. Karkamkar, J. Phys. Chem. C Lett. **113** 10319-10321 (2009).



Hydrides as new anodes for lithium batteries

The incorporation of lithium by hydrides through an electrochemical conversion reaction is a promising alternative to Li intercalation into graphite for next-generation Li-ion cells.

This reaction has been proved only for a couple of metal hydrides. We are currently studying the applicability of complex hydrides and possible improvements of the hydrides performances in the cells by means of artificial nanostructuring.



D. Meggiolaro, G. Gigli, A. Paolone, F. Vitucci, S. Brutti, J. Phys. Chem. C **117** 22467-22477 (2013).



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keywords

- Roe deer
- Distance sampling
- Levy flights
- Wild boar
- Capture-mark-recapture
- Mathematical, statistical modelling

Movement ecology

Movement ecology is an emerging ecological discipline whose aim is studying animals' movement in relation to their internal state, to the presence of conspecifics, competitors and predators and to the ecosystems complexity. The participation to the EURODEER working group allows to develop researches on movement of roe deer (*Capreolus capreolus*) thorough Europe with specific reference to migration, natal and reproductive dispersal and interspecific competitions

Levy flights

In the last 8 years a passionate debate about the presence of Lévy movements in wild animals has developed. To move forward it is necessary to develop new insight in searching behavior under field conditions, making use of the most innovative tracking device such as GPS tags. In particular we investigate the foraging behavior of shearwaters a bird species able to perform foraging excursions very far from their breeding colonies

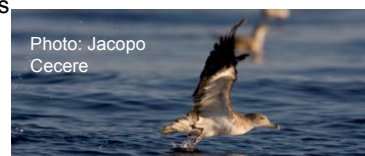


Photo: Jacopo Cecere

Population dynamics

Populations dynamics of wildlife is fundamental for our understanding of the dynamics of environments. The main target of this study is represented by the wild boar (*Sus scrofa*) and by its impacts on and relationships with natural and agricultural ecosystem.

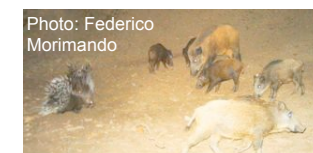


Photo: Federico Morimando

Population assessment

Effective monitoring of wildlife population is a basic need for cost-effective management and conservation. An effective method for population assessment is represented by nocturnal distance sampling, where animals are detected by night using thermal imaging. To be effectively implemented we develop a number of experiments under natural conditions in protected areas.

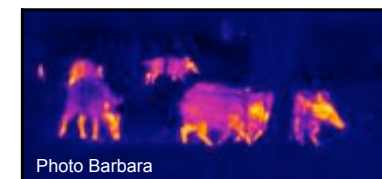


Photo Barbara



Andrea Gabrielli

Sapienza unit



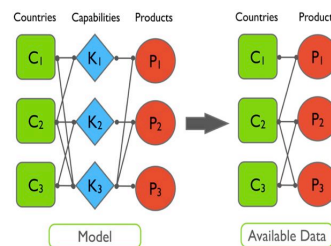
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keywords

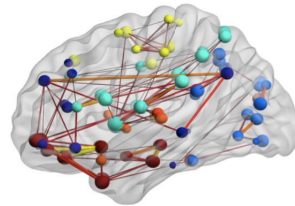
- Stochastic processes and networks for interdisciplinary applications
- Networks and complex structures in brain science
- Long range interacting systems

Economic complexity: If we study how different countries produce different products, we find data which look in contrast with standard economic theories: differentiation of production appears much more important than specialization for advanced economies. Studying the network structure of world production through a non-linear *pagerank-like* approach permits to uncover the hidden potential of growth of countries and to classify the technological complexity of products.



Complex structures in brain and NMR

Human brain is one of the most complex object of study in science and it is characterized by a spatio-temporal multiscale and multilevel structures. Nuclear Magnetic Resonance is the best *in vivo* tool to study both its 3-d disordered structure and its complex behavior. With this experimental technique, supported by the generalized diffusion theory, we can study the diffusion of water molecules in each cell (i.e. voxel) of a 3-d grid to get 3-d brain images (DNMR). The same technique is used to analyze the temporal coordination between different regions of the brain during its functioning (fMRI). Network theory then permits to determine the topological properties of this functional network and characterize in the best way the functional connectivity and coordinated behavior of different brain regions.



Quasi-stationary states in long range interacting systems

Particle systems with long range interactions (e.g. self-gravitating gas) present a peculiar behavior which differs strongly from standard short range interacting systems both at equilibrium (e.g. ensemble inequivalence, negative specific heat) and far from it. In particular their out of equilibrium dynamics is characterized by the presence of *quasi-stationary states* in which the system gets trapped. They are due to the prevalence of collective motion on the two-body collision dynamics which in general drives the system at equilibrium. Its study is still an open issue.



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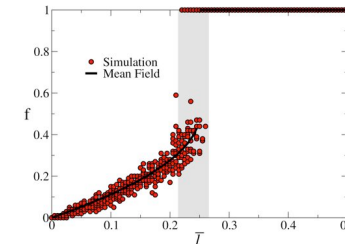
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keywords

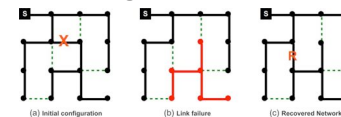
- Complex Networks: Critical Infrastructures, Social Networks
- Statistical Mechanics: Energy Landscapes, Soft Matter
- Computational Physics: Hard body simulations, Monte Carlo

Complex Networks and Power Grids



Electric power-systems are one of the most important critical infrastructures. We apply statistical mechanics to understand emerging phenomena in power grids

Self Healing Networks



We study self-healing models of complex networks modelling. Obvious applications are to infrastructural networks like gas, power, water, oil distribution.

Social Networks



We focus on data-driven computational models of complex socio-cognitive systems: spread of information and opinions, social human behavior, evolution of social networks. We aim to develop innovative mathematical models and computational tools to better understand, anticipate and control massive social phenomena with a complex systems approach.

publications

- **Abruptness of Cascade Failures in Power Grids**
Scientific Reports 4, 3694
- **Self-Healing Networks: Redundancy and Structure**
DOI: 10.1371/journal.pone.0087986
- **Opinion dynamics on interacting networks: media competition and social influence**
Scientific Reports 4, 4938



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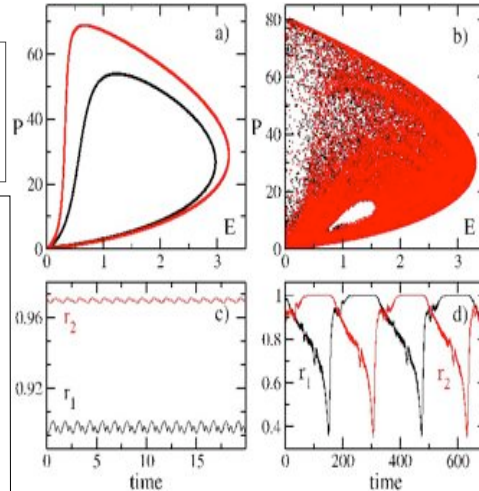
keywords

- *Neural Networks*
- *Phase Oscillators*
- *Out of Equilibrium Statistical Mechanics*

Dynamics of Massively Connected and Sparse Neural Networks

We have investigated the role played by the topology in promoting coherent activity in excitatory diluted pulse-coupled neural networks at a microscopic and macroscopic level. In particular, we considered a diluted random network where neurons were connected as in a directed Erdős-Rényi graph with average connectivity scaling sublinearly with the number of neurons in the network. In these "massively connected" networks we have shown that in the thermodynamic limit the dynamics of coherent collective states coincide with that of fully coupled networks. However, the random dilution of the connections induces inhomogeneities in the neuronal behaviors for any finite system size, promoting a weak form of chaos, which vanishes in the limit of infinite size. In this limit, the disordered systems exhibit regular (non chaotic) dynamics thus recovering the properties of a homogeneous fully connected network. The situation is quite different for a "sparse network" characterized by a constant connectivity, independent on the size of the network. In fact, on one side we found that a few tens of random connections are sufficient to sustain a nontrivial collective dynamics. In other words, collective motion is a rather generic and robust property and does not require an extremely high connectivity to be sustained. On an other side, the collective motion coexists with a microscopically chaotic dynamics that does not vanish in the thermodynamic limit and turns out to be extensive (the number of unstable directions is proportional to the network size). More specifically, various classes of dynamical models on random sparse networks have been studied and in all cases, irrespective of the presence of the macroscopic phase, we found that the chaotic dynamics is always extensive. Extensive chaos has been already found in spatially extended system with nearest-neighbour coupling (diffusive coupling) induced by the additivity of the system. In our case this property is highly nontrivial, as the network dynamics is non additive and it cannot be approximated as the juxtaposition of almost independent sub-structures.

S. Olmi et al., *Physical Review E* 81, 046119 (2010).
L. Tattini et al., *Chaos* 22, 023133 (2012).
S. Luccioli et al., *Phys. Rev. Lett.* 109, 138103 (2012).
S. Olmi and A. Torcini, *Scholarpedia* 8 (10), 30928 (2013).



Hysteretic transitions and chaotic chimera states in networks of Kuramoto oscillators with inertia

We performed finite size numerical investigations and mean field analysis of a Kuramoto model with inertia for fully coupled and diluted systems. In particular, we examined, for a Gaussian distribution of the frequencies, the transition from incoherence to coherence for increasingly large system size and inertia. For sufficiently large inertia the transition is hysteretic and within the hysteretic region clusters of locked oscillators of various sizes and different levels of synchronization coexist. A modification of the mean field theory developed by Tanaka, Lichtenberg, and Oishi [Physica D, 100 (1997)] allows to derive the synchronization profile associated to each of these clusters. By increasing the inertia the transition becomes more complex, and the synchronization occurs via the emergence of clusters of whirling oscillators. The presence of these groups of coherently drifting oscillators induces oscillations in the order parameter. We have shown that the transition remains hysteretic even for randomly diluted networks up to a level of connectivity corresponding to few links per oscillator. Finally an extension to a system of two symmetrically coupled networks of Kuramoto oscillators with inertia is analyzed. In this system the existence and the dynamical properties of novel chaotic chimera states are investigated, concentrating both on the microscopic dynamics and the macroscopic behavior.

S. Olmi et al., *Phys. Rev. E* 90 (4), 16 (2014).



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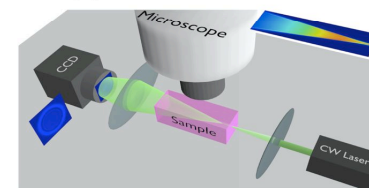
keywords

- *Random photonics*
- *Shock waves in complex systems*
- *Optomechanics*

The study of the propagation of light in complex nonlinear systems allows to observe a plethora of phenomena generated by the interplay between disorder and nonlinearity. Understanding such interplay furnishes insights of the fundamental mechanisms ruling the light transport regimes as well as opens the road to new applications in the field of the light-driven device.

Shock Waves

The dispersive shock waves (DSWs) are a nonlinear phenomenon, where the dispersion regularizes the occurrence of abrupt discontinuities by means fast coherent oscillations. Because their coherent nature, DSWs represent a suited candidate to experimentally investigate the competition between disorder and nonlinearity in complex materials [1].

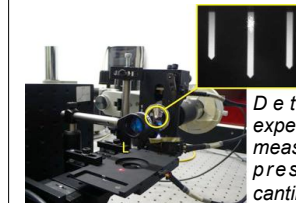


The DSWs have also provided the physical first realization of the inverted quantum oscillators. Such systems that were theorized by Glauber to explain the link between the reversible microscopic and irreversible macroscopic scale, represent nowadays a novel perspective to exploit shock-waves in useful applications as lasers, optical amplifiers and X-ray generation [2].

[1] N. Ghojaniha et al, PRL 109, 243902 (2012).
[2] S. Gentilini et al, Sci. Rep. 5, 15816 (2015).

Optomechanics

The concept of radiation pressure is based on the exchange of momentum between photons and matter. In recent theoretical studies a nonlinear opto-mechanical response is predicted and we experimentally measure thermal and electronic nonlinear effects. By means of an atomic force microscope (AFM) we are able to detect the nanometric deflection of cantilevers due to optical forces exerted by a continuous wave laser beam [3].

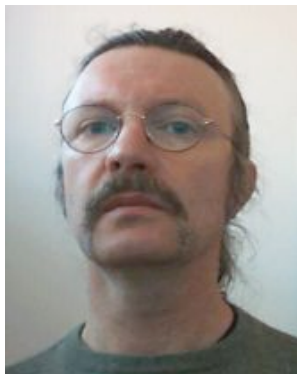


Detail of the experimental setup to measure the radiation pressure on AFM cantilevers [3].

We also theoretically consider the effect of light scattering on the opto-mechanical forces, finding that light trapping mechanisms enhance their action [4]. All these findings feed the exploitation of light for controlling motion of complex dielectric structures and realize light-activated devices

[3] C. Ciancio, Master degree thesis (2015).
[4] S. Gentilini et al., PRA 91, 043813 (2015).





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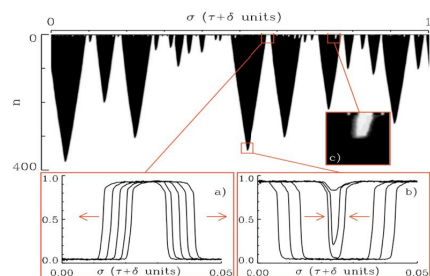
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keywords

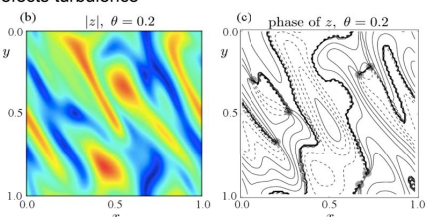
- Semiconductor laser physics
- Dynamical systems
- Stochastic processes

Dynamical systems with long delayed feedback

The correspondence between long-delayed systems and one-dimensional spatially-extended media enables a direct interpretation of purely temporal phenomena in terms of spatio-temporal patterns. On the basis of this result, we provide the evidence of a characteristic spatio-temporal dynamics -coarsening- in a long-delayed bistable system. Nucleation, propagation and annihilation of fronts, leading eventually to a single phase, are observed in an experiment based on a laser with opto-electronic feedback.

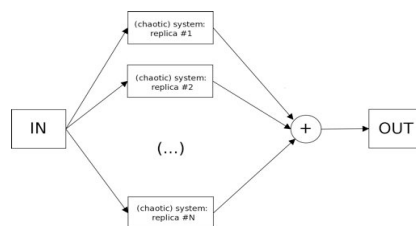


A class of systems with multiple, hierarchically long time delays uncover features otherwise hidden in their temporal dynamics using a suitable space-time representation. The behaviour in the case of two delays is shown to "encode" two-dimensional spiral defects and defects turbulence



Charactering the response of chaotic systems

We characterize the response of a chaotic system by investigating ensembles of, rather than single, trajectories. Time-periodic stimulations are experimentally and numerically investigated. This approach allows detecting and characterizing a broad class of coherent phenomena that go beyond generalized and phase synchronization. In particular, we find that a large average response is not necessarily related to the presence of standard forms of synchronization.



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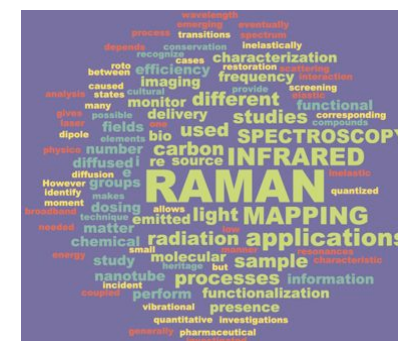
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keywords

- Vibrational Spectroscopy and Imaging
- Nanotechnology applied to Biomedicine
- Biosensors

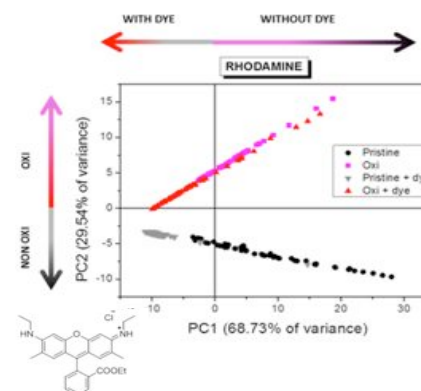
Tech4Bio

The inter-Institutes initiative Tech4Bio, collecting many researchers of CNR in Rome, is to promote the intersection between different disciplines, to provide a valuable opportunity to exchange information and expertise, to create connections and collaborations among researchers and to build a bridge between companies and places traditionally dedicated to frontier research. The group deals with biosensors and biochemistry, microscopy and spectroscopy, development of advanced microfluidic devices and lab-on-chips for Bioanalytics and Diagnostics, characterization at the micro and nano-scale, design and study of novel smart biomaterials.



PCA applied to Raman mapping for the rational design of functional nanostructures

Principal Component Analysis (PCA) can be applied to Raman mapping as a very robust method for a rapid and trusty classification of samples, which is fundamental to improve the design of functional nanostructures and to optimize the preparation procedure for the specific application. Such an approach has been recently applied to analyse the Raman maps collected on carbon nanotubes at different degree of oxidation and functionalization with various dye labeling molecules (results on Rhodamine shown on the left).





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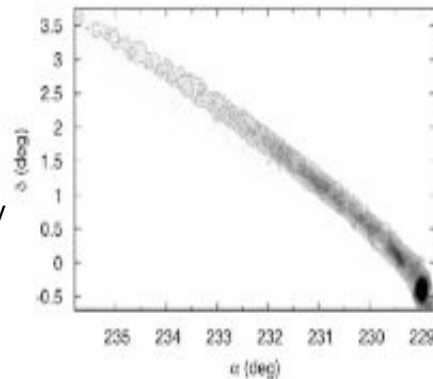
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<http://www.sapienza.isc.cnr.it/statistical-dynamics/statistical-cosmology.html>

keywords

- Globular Clusters dynamics
- Galaxy interactions

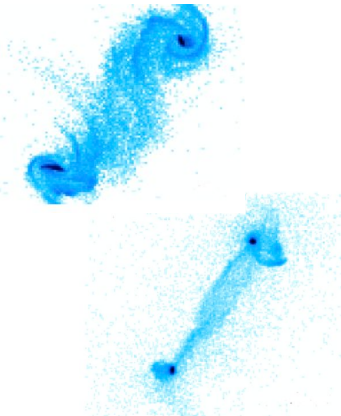
Globular Cluster dynamics

Globular Clusters (GCs) are old star clusters in the galaxy and cornerstone for our understanding of the formation, structure and dynamics of Milky Way. Last decade has seen the discovery of tidal tails emanating of GC. Tails are a new probe of the potential of the galaxy and its time evolution. Through numerical simulation and observational comparison we can explore the features of dark halo and its dynamics



Galaxy interactions

Galaxies are recognized as the product of evolution lasting nearly 14 billion years. It is clear that many galaxies interact with neighboring ones and galaxy interactions are believed to be the key evolutionary mechanism, in particular for the early-type. We are studying models and numerical simulations to understand which are the dominant physical processes which drives their evolution and produce the richness we observe in the universe



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keywords

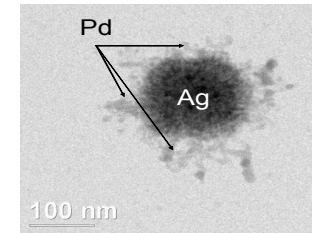
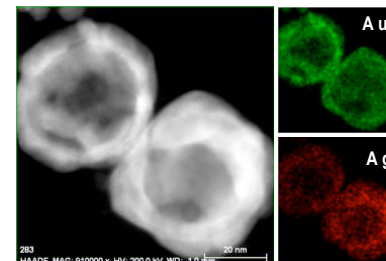
- Plasmonics
- Nanomaterials
- Laser ablation

Plasmonic nanomaterials for spectroscopic applications

Preparation and characterization of nanoparticles of coinage metals with tunable plasmonic properties (related to size and/or aspherical shape).

These nanoparticles cause Surface Enhanced Raman response (SERS) of molecular adsorbates and, under appropriate experimental conditions, also metal enhanced fluorescence (MEF).

Beyond enhanced spectroscopy, they can find application in novel sensing devices and in theragnostic (i.e. early detection and/or photothermal therapy of tumors).



Laser ablation

Laser ablation is a green physical approach to the production of nanomaterials. A pulsed laser beam is focused onto a target immersed in a liquid. The material extracted by laser-target interaction can aggregate into nanoparticles. This method permits to obtain stable metal colloids also in pure solvents, such as water. Under proper experimental conditions it can be used to prepare oxide and/or metal oxide or bimetallic nanoparticles. The nanoparticles can be unprotected, but also coated by different molecular adsorbates, when required. Among the wide range of applications, Ag colloids are interesting for their fungicide and bactericide properties, while Au or iron oxide colloids can find important applications in drug delivery systems and Pd colloids in catalysis.



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keywords

- Granular Materials
- Brownian Motors

Granular Materials

Granular materials are studied and used to test various fascinating theories in the field of non equilibrium statistical physics.

Many different experiments have been realized in the Granular Dynamics Laboratory in the Fermi Building, ground floor, Room 012. In our experiments grains are made of steel or plastic beads of various size, in the 1 – 4 mm range. The beads are kept in movement by a shaker and various different regimes are realized (granular gas and liquid) in various different setups (3d, 2d and also 1d). The dynamic of the grains is studied by high speed cameras and/or probed by intruders.



Brownian Motors

Brownian motors are a class of devices that extract useful work from noise. Such an extraction, which is impossible in the classical equilibrium thermodynamic framework, is made possible through the use of granulars that are, by definition, in non equilibrium conditions. The rectification of fluctuations is challenging from the experimental point of view and the final direction of motion is not easily predicted without a suitable theoretical model.



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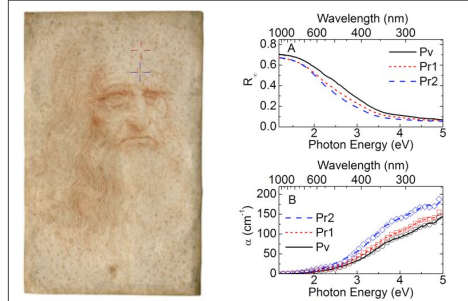
keywords

- Cultural heritage: degradation of ancient paper
- Ultraviolet-visible-infrared and THz spectroscopy
- Optical and structural properties of inhomogeneous systems

Optical degradation of ancient paper at the nanoscale

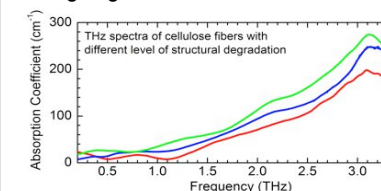
Yellowing of ancient paper is responsible for severe degradation of ancient artifacts. The study of this phenomena is complicated by the fact that paper sheets are inhomogeneous systems whose optical properties are strongly governed by light scattering effects. It is necessary to apply suitable experimental approaches and specific models for light propagation in turbid media in order to recover the optical spectra of compounds responsible for yellowing. Comparison with theoretical condensed matter computational simulations allows to describe and quantify at the nanoscale the modification of cellulose responsible for ancient paper visual degradation. This approach has been applied to the famous Leonardo Da Vinci's self-portrait [1]. New research activities are now on going to detect the degradation rate of this masterpiece and on other famous drawings of Leonardo. Research activities are carried on in collaboration with the Physics Departments of the University of Rome "Sapienza" and Tor Vergata, with the Chemistry Department of the University of Krakow, Poland, and with the Italian Minister for Cultural Heritage.

[1] A. Mosca Conte, O. Pulci, M.C. Misiti, J. Lojewska, L. Teodonio, C. Violante, and M. Missori "Visual degradation in Leonardo da Vinci's iconic self-portrait: A nanoscale study", Applied Physics Letters 104, 22, 224101 (2014)



Biological systems

Ultraviolet-visible-infrared and THz spectroscopy allow to study the optical and structural properties of non-homogeneous systems formed by biological fibers and biomaterials of medical interest and their interaction with water. Research work is also focused to the understanding of degradation phenomena of these materials caused by different aging factors (environmental, chemical, endogenous). Information recovered attracted the attention of companies and led to an ongoing collaboration.





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keywords

- Dissipative systems, metriplectic algebræ
- Near-Earth Plasma and Space Weather
- Mathematical Ecology

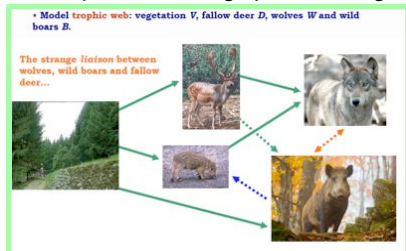
Metriplectic systems

Metriplectic formalism is a framework to turn dynamical systems with dissipation into algebræ of Leibniz brackets. In particular, when complete systems are dealt with, their entropy plays the role of generator of the dissipative irreversible component of motion. Many dissipative systems have been "algebrized" in this way: in particular, my contributions are on plasmas and fluids. Developments are expected in Quantum Mechanics.

- M Materassi, E Tassi, Physica D 241 (6), 729-734 (2012).
- M Materassi, Entropy 17 (3), 1329-1346 (2015).

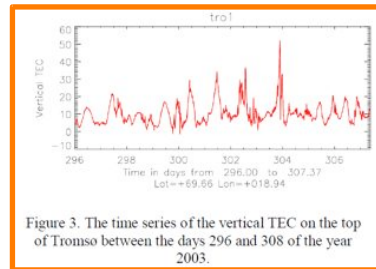
Mathematical ecology

Ecological webs are represented and studied through the population dynamics of the species composing them. My research is focused at the moment on scavenging and kleptoparasitism among big mammals, and competition among species of algæ.



Near-Earth Plasma and Space Weather

My oldest line of research is ionospheric dynamics, from the point of view of dynamical system theory. Participating to projects on Space Weather, I am studying the near-Earth plasma as a complex system forced and structured by the Sun's activity and the geomagnetic field. In this investigation there is room for multi-scale statistics of GPS signals, MHD reformulation via stochastic and fractal methods, and the use of information theory tools to detect causal relationships.



- A.W. Wernik, L. Alfonsi, M. Materassi, Radio Science 42 (1) (2007).
- M. Materassi, G. Consolini, Physical review letters 99 (17), 175002 (2007).
- M. Materassi, L. Ciraolo, G. Consolini, N. Smith, Advances in Space Research 47 (5), 877-885 (2011).
- M. Materassi, G. Consolini Journal of Plasma Physics 81 (06), 495810602 (2015).



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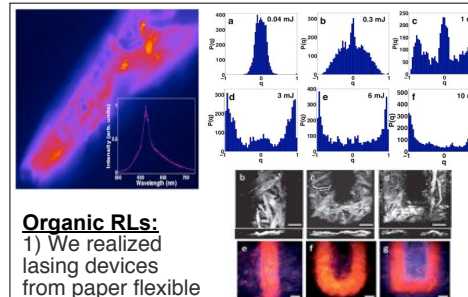
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keywords

- Random photonics
- Nonlinear waves
- Nonlinear optical properties of soft matter

Random Laser (RL) consists of a random assembly of scattering structures dispersed into an optical gain medium in which the optical cavity is merely represented by multiple scattering processes of light. In the last 20 years the research in RLs has provided important insights into some aspects of fundamental physics as Anderson localization and Bose-Einstein condensation and opened new routes towards the fabrication of innovative photonic devices.



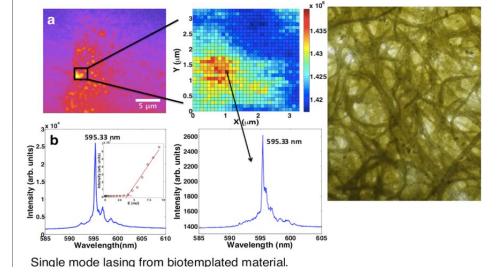
Organic RLs:

- 1) We realized lasing devices from paper flexible sheets by creating on the cellulose fibers **micro-fluidic porous channels** in which a fluorescent dye can flow by capillarity. We show how the emission properties depend crucially on the width, shape and curvature of the microchannels as well as on their functionalization with colloidal additives.
- 2) We observed tunable RL emission from scattering nano-aggregates of a **thiophene oligomer**, obtained in a controlled way by soft lithographic techniques. The emission from this organic dye in compact solid state showed the **experimental evidence of Replica Symmetry Breaking**.

- I. Viola et al. J. Mater. Chem. C **1**, 8128 (2013)
N. Ghofraniha et al. Opt. Lett. **38**, 5043 (2013)
N. Ghofraniha et al. Laser Photon. Rev. **7**, 432 (2013)
N. Ghofraniha et al. Nat. Comm. **6**, 6058 (2015)

Bio-templated RLs:

We observe **single mode lasing** emission from bio-mimetic materials. The transformations of the complete hierarchical structure of paper fibers into inorganic materials allow to obtain very efficient RLs with sub-nanometer lasing modes. We show that the distribution and the intensity of the modes change in different points of the system depending on the local structure of the material, in this way the RL emission can be used as a fingerprint of porous materials with high potentiality for example in medical diagnostics and cultural heritage. Moreover we demonstrate that resonant modes are extended in space, they interact and compete for the available energy. We plan experiments with other bio-inspired materials as diatoms, chitin fibers and graphene quantum dots.





Thomas Kreuz

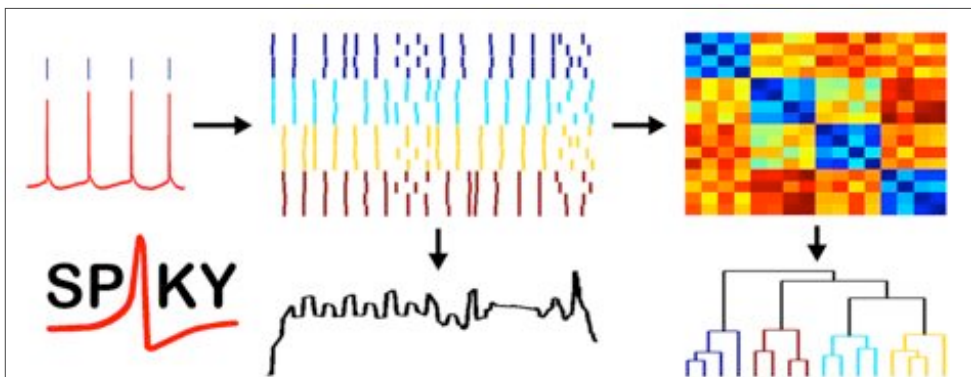
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keywords

- *Computational neuroscience*
- *Data analysis*
- *Measures of spike train synchrony*



Measures of spike train synchrony

In both experimental and computational neuroscience there is an increasing demand for algorithms capable of analyzing large amounts of spike train data. One of the most crucial tasks is the identification of similarity patterns with a very high temporal resolution and across different spatial scales. In recent years we have developed three time-resolved and parameter-free measures of spike train synchrony: The ISI-distance, the SPIKE-distance, and SPIKE-synchronization. In a second step we apply these measures to real neuronal data (medial temporal lobe of epilepsy patients, monkey retina, auditory system of songbirds etc.) kindly provided by collaborating laboratories.

SPIKY – Graphical user interface

SPIKY is a Matlab-based graphical user interface which facilitates the application of our time-resolved measures of spike train synchrony to both simulated and real data. SPIKY includes implementations of the ISI-distance, the SPIKE-distance and SPIKE-synchronization all of which have been optimized with respect to computation speed and memory demand. SPIKY also comprises a spike train generator and an event detector which makes it capable of analyzing continuous data. Finally, SPIKY includes programs aimed at the analysis of large numbers of datasets and the estimation of significance levels. SPIKY is complemented by the open source Python library PySpike hosted on github.



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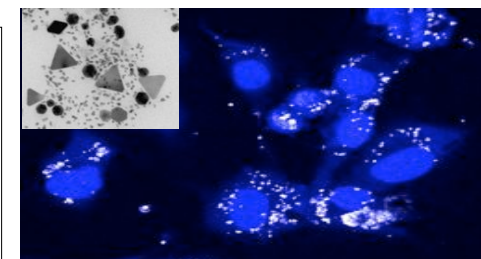
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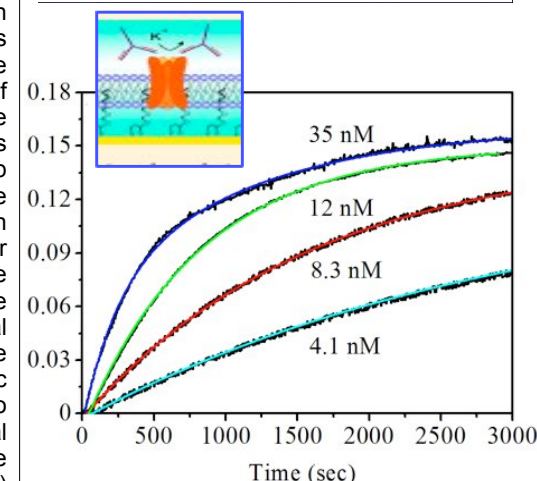
keywords

- *Plasmonics*
- *Metal Nanoparticles*
- *Plasmonic sensors*

Plasmonics is a field of Optics that deals with the interaction of optical beams with the free electrons of noble metals producing collective motions known as “surface plasmons”(SPs). The light-SPs interaction can provide a high intensification of light intensity at the metals interfaces, that become actually ideal sensitive tools to be exploited in several applications. The confined fields can be induced by a guided interface propagation or by dipolar or multipolar local resonances in nanostructures. In both cases, the phenomena are referred as “surface plasmonic resonances”. As the conditions for the resonant excitation of SPs strongly depend on the refractive index of the metal surroundings, this suggested a powerful way to develop sensitive physical-chemical, label-free sensors. This dependence has been exploited also in other fields, like non linear optics, or in the ultra-sensitive Surface Raman Enhanced (SERS), where the signals can be intensified up to several orders of magnitude with respect to the conventional Raman analysis.. Plasmonic localization is also an efficient tool to enhance the fluorescence emission (Metal Enhanced Fluorescence, MEF) or to excite the Multi Photon Luminescence (MPL) emission by metal nanoparticles.



Cell uptake of NIR-absorbing gold nanoparticles (white dots) emitting via MPL. Inset: triangles side ~50 nm



Surface plasmon resonance kinetics of the recognition by specific antibodies of potassium pumps hosted in bilayer lipid membranes





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keywords

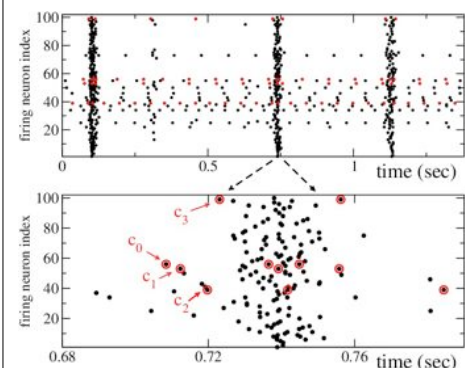
- Computational neuroscience
- Nonlinear dynamics and chaos
- Out-of-equilibrium processes

Functional Hubs Neurons

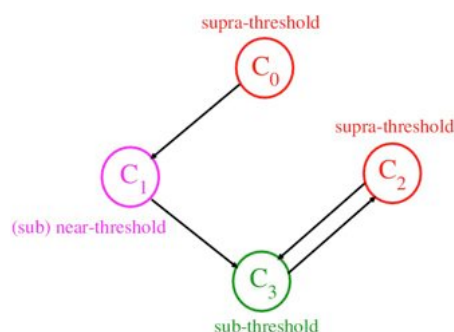
Recent experiments have shown that perturbations at the single neuron level can impact the overall synchronous dynamics of neural circuits. We study, by using realistic models, the emergence of self-organized pools of a few neurons (*cliques*), responsible for the triggering of the synchronous activity of the network. These neurons are *hubs* in a *functional* sense, as the played role is not related to the intrinsic degree of connectivity but to the sequential and coordinated order of spike emission preceding the synchronous event. The perturbation of even one single neuron of the *clique* can bring to the arrest of the collective synchronous activity of the network.

S.Luccioli et al PLOS Comp.Biol. 2014

Sequential activation of Hubs Neurons



Architecture of the clique



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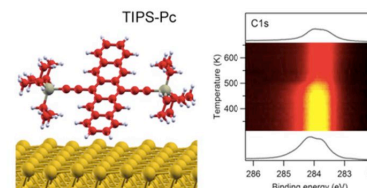
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keywords

- Properties of surfaces, interfaces and ultrathin films
- Graphene and 2D materials
- Surface reactions

Structural, electronic, and chemical properties of surfaces and interfaces.

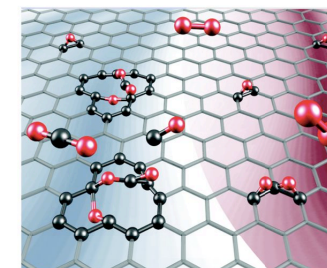
Most of the chemical and physical processes involving solid materials take place at the surface. These aspects become even more important for nanomaterials since the reduced dimensions make the surface rather than the bulk to dominate the physicochemical behavior. Therefore the knowledge of the interplay between the structural, electronic and chemical properties of the material surfaces is the key to optimize processes such as layer growth, interface formation, thin film synthesis, gas-solid interactions, catalysis, corrosion, oxidative reactions and gas sensing. We combine electronic, optical and microscopic diagnostics to investigate the intrinsic properties and the surface reactions triggered by external agents in nanostructured materials, organic/inorganic interfaces, ultrathin films and heterostructures.



Decomposition of TIPS-Pentacene on Au(111) monitored by fast XPS of the C1s core level. Ref. J. Phys. Chem C 18, 22522 (2014)

Growth and functionalization of 2D materials.

Due to its outstanding electronic, optical, morphological and mechanical properties graphene has opened up new horizons for the research and development of two-dimensional (2D) materials. These are materials that do not need to be supported by a substrate to exist and therefore can be isolated as free-standing one atom thick layers, and that due to confinement of electrons and to the lack of strong interlayer interactions usually exhibit optical and electronic properties different from their analogous 3D systems. Our research focuses on the development of methods to synthesize graphene and other 2D materials, to define their stability and understand how their properties are modified by doping and functionalization or by the formation of interfaces with dissimilar materials.



Graphene functionalized with O containing species. Ref. JACS 133, 17315 (2011)



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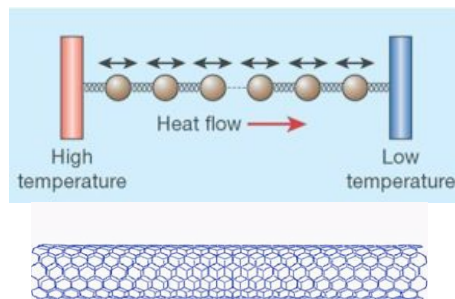
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keywords

- Non-linear dynamics and chaos
- Out-of-equilibrium processes in physics
- Fluctuations and random processes

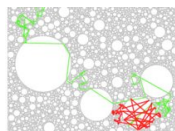
Anomalous heat conduction

Physical phenomena in reduced spatial dimension ($D < 3$) are often qualitatively different from their three-dimensional counterparts. An important example that has been thoroughly studied by our group is the anomalous heat conduction in chains of coupled oscillators. Numerical and analytical studies showed that correlations are so relevant to lead to a diverging thermal conductivity. This implies a breakdown of the usual hydrodynamic approach based on phenomenological constitutive equations (the Fourier law in this context). These ideas found recently applications in the framework of nanoscale heat transfer and has been tested experimentally for quasi 1D and 2D systems like carbon nanotubes and graphene.



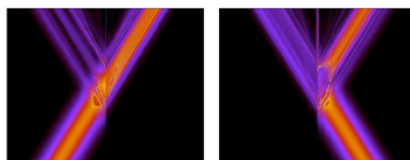
Diffusion on Levy structures

The effect of quenched, long-range correlated, disorder on anomalous diffusion has been studied. The powerful ideas of scaling has been employed to predict the transmission in engineered optical materials called "Levy glasses".



Asymmetric nonlinear wave transmission

Nonlinearity can lead to nonreciprocal transmission: the same wave is transmitted differently in opposite directions. Different regimes of scattering can exist such as nonreciprocal modulation via Hopf bifurcations of the steady solutions and a regime of a "chaotic diode", where transmission is regular in one direction and chaotic in the opposite one.



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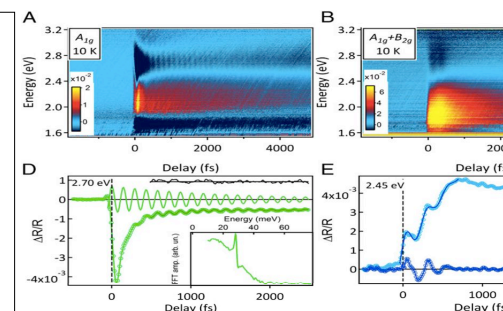
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keywords

- Theory of Many-Body Systems
- Superconductivity
- Emerging materials

Complex Solids

My main interest are complex solids intended as materials in which different phases compete producing interesting collective behavior. Competition arises because interactions and the kinetic energy contribute similarly to the energy, therefore complex solids are not in the weak nor in the strong coupling regime which makes them difficult to treat with conventional perturbative approaches. Competition between phases often leads to gigantic responses to external perturbations which makes complex solids interesting for applications. I use many-body numerical and analytical techniques to model the behavior of systems with fascinating properties as high temperature superconductors and multiferroics (materials which have ferroelectric and magnetic order coupled). My work is often close to concrete experiments performed by partner groups and in the last years have been focused on time-dependent phenomena as collective modes of superconductors (including the possibility to observe the analogous of the Higgs boson in condensed matter), generation of magnetic responses with an electric pulse or vice versa and understand the physics of many-body quantum systems out of equilibrium.



Many-body physics in real time

In the last years dramatic technical progress has enabled experiments where quantum matter is perturbed and its evolution is monitored in the femtosecond time scale. The figure shows experiments by our partners at Lausanne [Mansart et al. PNAS, 110, 4539 (2013)] where the reflectivity as a function of energy is monitored as a function of time delay after an impulsive perturbation. Ultrafast time resolution allows to see lattice vibrations (A and D) and also electronic oscillations (B and E). The material is a high temperature superconductor and the electronic oscillations are attributed to the superconducting condensate. Modeling these and related experiments can help to understand the mechanism of superconductivity in these materials, one of the main open problems in physics.