# Physics of Complexity @ISC

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institute for complex systems

C 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, October 2017

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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 undirectional rotational motion when immersed in a bath of selfpropelled 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.



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

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.

[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)



glass-glass transition [2].





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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.



Sapoval, B., Baldassarri, A., & Gabrielli, A. (2004). PRL, 93(9), 98501.

### 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 frictional response of a granular material could be very fluctuating, due to the anomalous stress propagation in the material. It represents an interesting experimental and theoretical problem, possibly connected to the physics of earthquakes.

Baldassarri, A., Dalton, F., Petri, A., Zapperi, S., Pontuale, G., & Pietronero, L. (2006). PRL, 96(11), 118002.

#### Avalanche dynamics and crackling noise

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



Baldassarri, A., Colaiori, F., & Castellano, C. (2003). PR, 90(6), 60601.



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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 **competitio** n 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. Lemarie et al. Phys. Rev. B 87, 184509 (2013). In analogy with its counterpart in the Standard Model, in superconductors a collective Higgs boson emerges in the broken-symmetry state. It is formed by collective electronic excitations of the order-parameter amplitude. However, such a bosonic collective mode interferes dramatically with the underlying fermionic quasiparticle excitations, which control its dynamical properties and its coupling to external probes. This has crucial consequences on its observability in equilibrium and out-of-equilibrium spectroscopy, a topic under intense investigation in the current literature.



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

- 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

- 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 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, 91, 012808 (2015).

# 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.



#### TI

processes in the social domain, spurred by 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).

C. Castellano, R. Pastor-Satorras, "Topological determinants of complex networks spectral properties: structural and dynamical effects", Phys. Rev. X (in press).



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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 amorphuos 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



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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 andSimulations,StatisticalMechanics.MechanicsStatistical

# 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.





#### 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 led 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, strango attractors and the

strange attractors and the related fractal structures.

Fig. A strange attractor showing a fractal structure.





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keywords

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

#### Transport of swimming microorganisms in turbulence

Substances transported by a turbulent flow typically mix quickly (e.g stirring milk into coffee). What does happen to **microorganisms 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 or remain trapped in shear flow.** 



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)

F. Santamaria, F. Lillo, M. Cencini, G. Boffetta, Physics of Fluids 26, 111901 (2014)

M. Cencini, M Franchino, F Santamaria, G. Boffetta, J. Theor. Biol. 399, 62 (2016)

#### Time irreversibility in turbulence

We recentely investigated Irreversibility of Lagrangian dynamics in turbulence showing that its statistics can be rationalized within the multifractal model of turbulence



M. Cencini, L. Biferale, G. Boffetta and M. De Pietro arXiv:1707.08837 [physics.flu-dyn]

#### Neutral biodiversity models

Macroecological patterns, such as species abundance distributions and 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, e.g., to microorganisms ecology. We also considered near neutral models to assess the role of other effects.

S. Pigolotti and M. Cencini J. Theor. Biol. **260**, 83 (2009)

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

- S. Pigolotti, M. Cencini
- J. Theor. Biol.338, 1 (2013)



A recent review S. Pigolotti, M. Cencini, D. Molina, M. A. Muñoz arXiv:1708.03475 [q-bio.PE]



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keywords

- Network Science
- Dynamics of Social Systems
- Epidemics Phenomena

Interdisciplinary research Physics as a tool

### topics

#### General setting

<u>Complex systems</u>: in many diverse systems an emergent macroscopic behavior arises from simple interacting units.

<u>Network science</u>: the topology of the network of interactions is common to many apparently unrelated systems, and plays a crucial role in the emergent behavior. Understanding the contact network structure is a key issue, transversal to many interdisciplinary applications.

#### Dynamics of social systems

Many large-scale phenomena observed in social systems are emergent behaviors produced by a large number of interacting individuals. They can be studied in terms of statistical physics models borrowing concepts and tools from physics. Dynamical processes are generally well studied on regular lattices, however, in complex systems, the peculiar topology of the contact networks deeply affects the dynamics upon them.



Spreading processes are typical dynamical processes in social systems. Examples are information diffusion or meme propagation, opinion dynamics, language evolution, or infectious disease epidemics. In all these cases the nontrivial topology of the network of interactions strongly impacts the emergent behavior.

#### **Typical questions**

In social contagion: What are the mechanisms leading to consensus? What makes a minority resilient, allowing plural opinions to survive? What causes an opinion shift? What makes such a shift abrupt? What is the weight of peer pressure w.r.t. an external influence such that of media? When unfavored opinions might gain the support of the majority? In infectious disease epidemics: Can we predict disease outbreaks and design effective strategies to prevent them? What characteristics of the contact network determines efficient vaccination strategies? What happens when multiple pathogens or multiple strains simultaneously propagate in the same host population?

methods

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



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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 biotemplated 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

- Roe deer
- Distance sampling
- **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 partecipation 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



- Levy flights
- •Wild boar

Capture-mark-recapture

#### **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 agricoltural ecosystem.

Mathematical, statistical modelling



### **Pupulation 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.





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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 mages (DNMR). The same Countries Capabilities Products Countries Products  $C_1$   $K_1$   $P_1$   $C_1$   $P_1$   $C_2$   $K_2$   $P_2$   $C_2$   $P_2$   $C_3$   $K_3$   $P_3$   $C_3$   $P_3$ Model Available Data



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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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].

N.Ghofraniha et al, PRL 109, 243902 (2012).
 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.Ciancico, Master degree thesis (2015).[4] S.Gentilini et al., PRA 91, 043813 (2015).



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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 longdelayed 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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### 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 lasertarget 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 opxide colloids can find important applications in drug delivery systems and Pd colloids in catalysis.



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keywords

- Soft matter: simulations and theory
- Effective interactions, phase diagrams and arrested states

### **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, heterogenous surface) or by varying externally the conditions of the solutions in which they are suspended. In this way, they experience effective interactions mediated by the solvent and show phenonema 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 cosolutes, unusual effects can be found. For instance novel effective interactions can be found when cosolute particles are (I) close to a critical point (ii) close to percolation (iii) close to the liquid-nematic transition. My research focuses on investigating novel mechanisms to induce effective interactions in colloidal solutions by means of numerical simulations.



Effective interactions of two colloids (gray) particles (I) in the absence of co-solute (ii) with non-interacting hard-sphere co-solute (iii) with chain-forming co-solute (iv) with pre-critical co-solute

N. Gnan et al. Soft Matter 8 (2012) N. Gnan et al., Nat. Comm.. 5, 3267 (2014) L. Rovigatti, N.Gnan et al. Soft Matter 11 (4), 692 (2015) N. Gnan. et al. Soft Matter 12, 9649 (2016) N.Gnan et al. Soft Matter 13, 6051 (2017)

#### Modeling Microgels



Microgels are soft particles individually made by cross-linked polymer networks which are widely used as a colloidal model system thaks to their swelling properties and their responsivity to external control parameters such temperature or pH. Their internal architecture affects the effective interactions between microgels, especially at high densities, where the polymeric nature of the particle becomes important due to strong interpenetration and entanglements. To go beyond the simple models available so far we have recently synthesized microgels in-silico using different preparation protocols. The aim of the research is to design and investigate numerically, coarse-grained microgels with properties comparable to the experimental ones.

N. Gnan et al, Macromolecules (2017) dx.doi.org/10.1021/acs.macromol.7b01600

### Glass Transition in soft matter

Part of my research is devoted to the study of dynamic and structural signatures of the glass transition in soft matter systems such as emulsions, core-shell particles, microgels etc...

N. Gnan et al. JSTAT (9), 094003 (2016) N. Gnan et al. PRL.110 (3), 035701(2014)



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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

- 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 tibers **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 Simmetry 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.





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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 SPIKEdistance, 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 ISIdistance, the SPIKE-distance and SPIKEsynchronization 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.



### **Rosanna Larciprete**

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keywords

Properties of surfaces, interfaces and ultrathin filmsGraphene 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 heterostrucures.



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 twodimensional (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. Rif. JACS 133, 17315 (2011)



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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 gualitatively different from their three-dimensional counterparts. An important example that has been thorughly 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 idea found recently applications in the framewok 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 I: 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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keywords

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

#### **Quantum Complexity**

My main interest is 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 nor 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, 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 timescale. The figure shows experimental results from a collaboration with our partners at Laussane [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.



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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 selforganized 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 supra-threshold $C_1$ supra-threshold (sub) near-threshold $C_3$ sub-threshold





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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

- 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 algeb ræ 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 kle ptoprasitism 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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### keywords

- Biofluids and macromolecular dynamics
- Physiological flows

#### Macromolecular motion

Proteins, DNA, lipids show a non-trivial intrinsic dynamics and a complex response to external flow conditions. In this respect, theoretical frameworks allow investigating large crowds of macromolecules and their time evolution. Numerical simulations unveil how dynamics takes place ranging from single-molecule to collective behavior, as pertinent to systemic biological response.





#### **Complex biofluidics**

The transitions of proteins as much as the formation of large biomolecular aggregates takes place under special external conditions, as for the catchbond proteins or for the coagulation cascade. Given the multiscale nature of these processes, high-performance simulations offer a privileged microscope to understand how flow, structural heterogeneity and chemical recognition work together to establish complex biological function.





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keywords

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

# Degradation of ancient paper at the nanoscale

The study of this phenomena is complicated by the fact that paper sheets are inhomogeneous systems. This affects the optical properties which 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 visual degradation. Comparison with ab-initio computational simulations allows to describe and quantify at the nanoscale the chemical modification of cellulose responsible for visual degradation. This approach has been applied to the famous Leonardo Da Vinci's self-portrait [1]. Research activities are also focused to the mapping the morphological and nano-mechanical properties of cellulose fibers at the nano-scale by using atomic force microscopy.

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, with the Italian Minister for Cultural Heritage and with companies .

[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)

[2] L. Teodonio, M. Missori, D. Pawcenisc, J. Łojewska, F. Valle "Nanoscale analysis of degradation processes of cellulose fibers", Micron 91, 75–81 (2016).



# THz spectroscopy of complex systems

THz spectroscopy allow to study the structural properties of non-homogenous systems formed by biological fibers and biomaterials of medical interest and their interaction with water. Research work is focused to the understanding of degradation phenomena of these materials caused by different aging factors (environmental, endogenous). THz spectroscopy is also applied to probe aqueous solutions of ions in order to characterize the dielectric properties of the solvent in the THz frequency range.





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### keywords

Evolution and dynamics of galaxies

#### **Milky Way evolution**

The Milky Way as other galaxies, is an evolving system, due to internal and environmental processes as well. There is not a unique process for the formation of different galactic components, but very likely several process at (maybe ?) different times. Through numerical simulation and observational comparison we are exploring the formation and evolution of Milky Way



From Purcell et al 2011



#### **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

- 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 pulsecoupled neural networks at a microscopic and macroscopic level. In particular, we considered a diluted random network where neurons were connected as in a directed Erdös-Renvi 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 suffcient 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).



## Antonio Scala

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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

- Spectroscopies
- Innovative materials for energy storage
- Ionic liquids

The design and development of systems for energy storage and conversion, from batteries to fuel cells, require new and more performing materials. We use a combination of complementary experimental and computational techniques, to achieve a detailed understanding of the structural and dynamical properties of these materials.

Ionic liquids (ILs) show properties that make them suitable electrolytes for elctrochemical devices. These macroscopic properties are strictly related to the microscopic configurations of anions and cations, which can be studied by combining abinitio simulation and infrared spectroscopy. In particular, we proposed that the competition among possible anion conformers can be the origin of the lack of crystalline phases in mixtures of different ILs and can be exploited as a valid tool to tailor the physical properties of the lack of the lack

> O. Palumbo et al. Phys Chem Chem Phys 19, 8322 (2017)

O. Palumbo et al. J Phys Chem C 121, 11129 (2017)



An experimental setup was developed to measure the mechanical modulus of ILs and its variation during the main phase transitions occurring by varying the temperature, in both the liquid and the solid states. These measurements, combined with DFT calculations, provide information about the dynamics and kinetics of ions. As an example, we revealed a relaxation attributed to the ions motion, which can be described by a hopping model between nonequivalent configurations, identified by the anion conformers them B 119 12905 (2015)O. Palumbo et al J Mol Liq 243, 9 (2017)





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keywords

- Spectroscopies
- Innovative materials for energy storage
- Ionic liquids

The design and development of systems for energy storage and conversion, from batteries to fuel cells, require new and more performing materials. We use a combination of complementary experimental and computational techniques, to achieve a detailed understanding of the structural and dynamical properties of these materials.

Due to their peculiar properties, ionic liquids (ILs) generate lot of interest for their possible use in a wide range of areas including catalysis and electrochemistry. The concentration of the ion configurations as a function of pressure and temperature can be studied by vibrational spectroscopy and provides informations about phase transitions and the nature of the intermolecular interactions. The exploration of an extended p–T region allows us to draw general remarks on the phase diagram of ILs.



A Paolone et al. J Phys Chem B 120, 2921 (2016) A Paolone et al. J Phys Chem B 120, 1312 (2016)

Ni-Nb-Zr amorphous alloys are proposed as new hydrogen permeation membranes to separate H  $_2$  from CO  $_2$ and other gases obtained from water shift reaction of coal-derived syngas.. Volumetric method combined with differential thermal and dynamical mechanical analysis allow the study of their hydrogenation properties. These information are fundamental, since the formation of hydrides can lead to eventual failure of the membrane.



A. Paolone et al. Energies 8, 3944, (2015). S. Sarker et al. Appl. Phys. A 122, 168 (2016).





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### keywords

- Granular matter
- Disordered materials
- Out of equilibrium critical systems

#### **Dynamics of granular matter**

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, dissipative processes and slow dynamics.



We try to improve our understanding of granular collective dynamics by means of laboratory experiments, numerical simulations, and look for stochastic processes suitable to describe it.





**Out of equilibrium criticality** Structural phenomena occurring in disordered materials often bring the features of criticality, i.e. long range correlations and self similar patterns, like for example a propagating crack. Despite their complexity, it is often possible to understand many features of these phenomena by means of simple models like cellular automata and lattice gases.



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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 composit boson formalism is then necessary to study polariton-polariton scattering in semiconductor microcavities. *L. Pilozzi et al. Phys. Rev. B 82, 075327 (2010) M.M.Glazov et al. Phys. Rev. B 80, 155306 (2009)* 

### Subwavelenght 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.

Phys. Rev. B 86, 045301 (2012)

L. Pilozzi et al.





#### **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 selfsimilarity 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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keywords

- Complexity in low dimensional magnets
- Molecular magnets (clusters and chains)
- Ultrathin magnetic films

# The classical and quantum dynamics of molecular spins on graphene

We explored the spin–graphene interaction by studying the classical and quantum dynamics of Fe4 magnetic molecular clusters grafted on graphene. Whereas the static spin properties remain unaltered, the quantum spin dynamics of the hybrid system are profoundly modified. For T<1K, the coupling of molecular spins to graphene electrons introduces a resonant quantum tunneling, with a reduction of six orders of magnitude in the spin relaxation time  $\tau$ .



# Rotatable anisotropy in thin magnetic films

In certain classes of thin ferromagnetic films, the in-plane magnetization direction is completely isotropic, nevertheless there is an effective energy barrier opposing the free in-plane rotation of the magnetization. Such in-plane "rotatable" anisotropy arises from the competition between a moderate amount of single-ion perpendicular magnetic anisotropy and the long-range easy-plane dipole-dipole coupling. We explored this phenomenon in ion-irradiated FePt films, presenting both isotropic inplane remanence and finite energy gap.



S. Tacchi et al., Phys. Rev. B **94,** 024432(2016) doi: 10.1103/PhysRevB.94.024432

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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, a system *driven* far from equilibrium or an active matter system may display some common features: the instability of an homogeneous state, the rising of a new structured state and the adjustement 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. Another, completely different example is given by the dynamics of the Discrete Nonlinear Schroedinger equantion (DNLS), which describes wave propagation in nonlinear lattices and which shows a ``negative tmperature" regime where localized excitations (breathers) appear and whose dynamics is essentially frozen because relaxation times diverge exponentially with the size of structures.





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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.



### **Belief Propagation**

A lot of *statistical-inference problems* of high technological importance (for instance: errorcorrection 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 statisticalmechanical method of the mean field type (Bethe-Peierls approximation).



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kevwords

- 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 smallsized 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-longitudinalmode 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 multilongitudinalmode 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 belowthreshold 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

- 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-ofequilibrium 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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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

- 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:



#### 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, thermoand 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).



Multiangle DLS



Multispeckle DLS



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### keywords

- Non-Equilibrium Statistical Mechanics
- Granular and Disordered Systems
- Brownian Motors and Anomalous Diffusion

#### **Non-Equilibrium Statistical Mechanics**

Systems out of equilibrium are characterized by the presence of currents (of energy or matter) and by dissipation. For these systems some results of standard statistical mechanics can be extended, such as the fluctuation-dissipation relation, but a general theory is still lacking. My interest is focused on the study of fluctuation theorems and fluctuation-dissipation relations in stochastic models.

Phys. Rev. Lett. 112, 140602 (2014) PLOS ONE 9, e93720 (2014) Phys. Rev. E 78, 041120 (2008) Phys. Rev. E 81, 011124 (2010)

#### Granular systems

Granular systems are heterogeneous conglomerations of macroscopic grains that interact via inelastic collisions. They present non-trivial rheological properties under external perturbations, and can show solid-, fluid-, or gas-like behaviors.

I study some models of granular media where a hydrodynamics description can be useful to describe the collective phenomena arising in these systems.

EPL 92, 34001 (2010), EPL 96, 14004 (2011) J. Stat. Mech. P08017 (2011)



#### **Brownian motors**

Molecular motors are systems that convert energy into directed motion. I study simple models where non-equilibrium conditions and spatial asymmetry induce a motor effect, in the presence of frictional forces. Phys. Rev. Lett. 110, 120601 (2013) Phys. Rev. E 88, 052124 (2013)

I also study the dynamics of driven tracers in crowded environments, which shows anomalous behaviors. Phys. Rev. Lett. 117, 174501 (2016) Phys. Rev. Lett. 115, 220601 (2015) Phys. Rev. Lett. 113, 268002 (2014)



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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

- 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, electrophoresys and microscopy techniques, we investigate the self-assembly phenomena occurring in co-suspension of



#### 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 fenomena 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

- Anomalous diffusion in confined systems
- Biophysics: cancer physics, cell and polymer conformational dynamics
- Failures in brittle and plastic materials

#### **Cell bleb dynamics**

Cells programmed to die undergo what's known as blebbing: the thin layer of crosslinked biopolymers underlying the membrane ruptures, causing it to bulge outwards in transient fluid-filled protrusions. These shape changes are thought to be driven by pressure-induced flow inside the cell without modifying its volume. We have observed fluid transport through the membrane of migrating stem cells, providing experimental and numerical evidence of marked reduction in bleb activity when this flow is hindered, and a correlation between surface and volume fluctuations.

A.Taloni *et al.* Phys. Rev. Lett. **114**, 208101 (2015). Research Highlights. Nature Physics **11**, 443 (2015).





# Thermally activated brittle fractures

The idea that the solid failure can be described by means of the Kramer theory, where the intrinsic energy barrier is reduced proportionally to the applied field, first appeared in material science to treat the kinetic fracture of solids under applied stresses and dates back to '40s. Starting from recent theories developed for single-molecule pulling, we have generalized the extreme value theory to account for failures of materials with an explicit dependence on temperature, strain rate and size of the object. This theory successfully applies to several experimental data and simulations on defected graphene sheets.

A.Sellerio et al. Phys. Rev. Appl. 4, 024011 (2015).





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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 Superieure, 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, Imparato 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 simmetry 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

- 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





# 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.





### **Ruggero Vaia**

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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 looses its coherence. However, if the array's bonds (i.e., sping 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 gubits, which is one of the basic tasks that a quantum computer based on gubits 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<sup>-1/6</sup>, 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.





The proposal consists in a system of atoms with two internal states trapped in a onedimensional 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

- 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 guantum 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 guantum 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 spinchain** (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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### 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: <u>Evidence from a field study</u>
   Proceedings of the National Academy of Sciences 105 (4), 1232-1237
- <u>Collective Behaviour without Collective Order</u> <u>in Wild Swarms of Midges</u> 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.

- <u>Silent Flocks</u> 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 ;
- <u>Scale-free correlations in starling flocks</u> Proceedings of the National Academy of Sciences 107 (26), 11865-11870
- <u>Statistical mechanics for natural flocks of birds</u> Proceedings of the National Academy of Sciences 109 (13), 4786-4791





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keywords

- Soft matter: simulations and theory
- Effective interactions, phase diagrams and arrested states

### erc MIMIC & MODELING MICROGELS: FROM MICROSCOPIC DESIGN TO MACROSCOPIC DESCRIPTION

Microgels are colloidal-scale particles individually made of crosslinked polymer networks that can swell and deswell in response to external stimuli, such as changes to temperature or pH. The size responsivity of microgels allows tuning the particle volume fraction of the system without changing the particle number density, and hence to explore soft matter physics in novel ways. The most studied microgels are based on PNIPAM etworks, which are thermoresponsive and display a volume phase transition at temperature T ~  $32^{\circ}$ C, from a swollen state at low T to a compact state at high T.

My research work is mainly focused to address these problems by performing numerical simulations of microgels in several situations starting from a single particle description able to capture the important features of experimental microgels, in collaboration with experimental soft matter group @CNR -ISC and with Lund University, Sweden.

*To read more see our recent work:* N. Gnan, L. Rovigatti, M. Bergman, EZ dx.doi.org/10.1021/acs.macromol.7b01600 **Selected as ACS Editor's Choice** 



#### **Objectives of MIMIC research project:**

**1)** To synthesize *in-silico* coarse-grained microgel particles with the correct swelling behaviour and elasticity;

2) To obtain accurate effective interactions between monomer-resolved microgel particles;
3) To predict the structure, dynamics, and rheology of bulk microgel suspensions, based on these effective potentials, and compare the results with experiments and existing theories.



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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.





### For further information please visit the website

#### www.isc.cnr.it

