Sapienza
Università di Roma

Dipartimento di Scienze di Base e Applicate per l'Ingegneria

Scientific Report
2018 – 2020

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Scientific Report 2018 – 2020

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Technical support by A. Belardini and A. Schiavi

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Introduction

I am very pleased to introduce the 2018–2020 Scientific Report of the Department of Basic and Applied Sciences for Engineering (Dipartimento di Scienze e di Base e Applicate per l'Ingegneria, SBAI).

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Research Activities: Chemistry

Chemistry-Introduction

The knowledge of any artificial and natural process involving Material Science and Technology, which covers a crucial role in the current development of each country, requires skills and expertise of Chemists.
In this context, we briefly describe in this Introduction how chemists in our Department (SBAI) combine their expertise in the Fundamentals of Chemistry (the basic principles taught in the School of Civil and Industrial Engineering) with some among the most promising and attractive "hot topics" studied in the recent years (mainly related to Material Science).

These issues are listed as follows: applied electrochemistry (concerning materials for batteries or organics for electronics, production of hydrogen, study of the antioxidant properties of phenolic compounds), ionic liquids (as solvents, or electrochemical precursors, or to analyze the competition between vaporization and decomposition), structural, morphological, electrochemical and thermal characterization of inorganic, organic and hybrid materials.

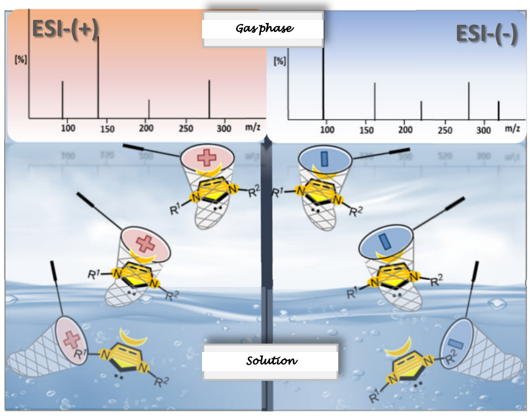
The equipment of diagnostic instrumental techniques of the Chemists belonging to the SBAI Department is related to the following techniques: X-ray Diffraction Powders (XRDP), Scanning Electron Microscopy (SEM), UV-Vis, NMR and FTIR spectroscopies, Liquid Chromatography (LC) coupled to Mass Spectrometry (MS), Thermogravimetry (TG), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC), operating simultaneously (TG/DTA or TG/DSC).
A fruitful collaboration with Consiglio Nazionale delle Ricerche and Centro Ricerche Casaccia of the Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile (ENEA) is still active since many years. On the other hand, any form of collaboration with Italian and foreign colleagues including sharing the mentioned equipments are welcome.

As far as the period 2018-2020 is concerned, chemists of SBAI were mainly involved in the area of Applied Electrochemistry, with particular reference to the study of ionic liquids and production and storage of energy, lithium-ion batteries, chemical synthesis of organic materials for electronics, redox properties of potential antioxidants. Other promising themes investigated include the electrochemical synthesis of nanostructurated materials for energy applications, and the thermal, structural and morphological characterization of gel-glasses, organic-inorganic hybrids, plastic waste as well as the thermodynamic and kinetic study of novel ionic liquids.

Task-Specific Ionic Liquids & Ionization Mass Spectrometry: studies to highlight the reaction mechanisms

Ionic liquids (ILs) represent a fascinating class of stable compounds that, owing to their recyclability and ignorable vapour pressure, are commonly used as green solvents in a variety of chemical reactions. We have studied the possibility to incorporate suitable functional groups into the cationic or anionic scaffold allows one to implement their catalytic properties and design task-specific derivatives for synthetic applications. The Knoevenagel condensation between an aldehyde and an activated methylene compound provides an archetypal example of chemical reaction in which the employment of a well-designed basic catalyst can be useful to optimize the selectivity of the process. Likewise, the elucidation of the reaction mechanism is essential to finely design the features of the catalytic system, although it is often hindered by the instability of the elusive intermediates that prevents their isolation and characterization. To this end, the high sensitivity and speed of the electrospray ionization mass spectrometry (ESI-MS) have been exploited in this study to efficiently intercept the ionic reactants, intermediates and products of the Knoevenagel condensation, characterize them by collision-induced dissociation (CID) experiments and highlight the action mechanism of task-specific ionic liquid the 1-methyl-3-carboxymethylimidazolium chloride (MAICl) as reaction catalyst.

To shed light on the mechanistic picture, the reaction mixture was sampled after different prefixed times and analysed by electrospray ionization mass spectrometry in both polarities. The mechanistic picture was highlighted and experimentally verified for different substrates and catalysts. [1]



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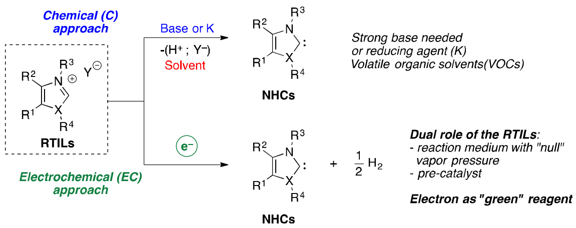
Ionic Liquids: not only solvents in electrochemistry

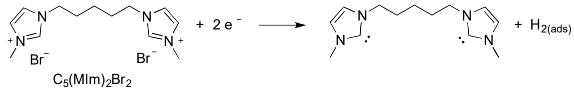
Ionic liquids (ILs), salts constituted of a large organic cation and an organic or inorganic anion not coordinated (usually liquid below 100 °C), are gaining more and more popularity in many fields of Chemistry. Due to their physico-chemical properties their use is advantageous in view of a “greener” way of thinking Chemistry although there are not sufficient studies on their possible toxicity. [1] In particular, their high solvation ability, their virtually null vapor pressure, the relative easiness in removing them from the reaction mixture and recycle them, spurred chemists to revisit established chemical reactions using them both as solvents and as reagents. Imidazolium ionic liquids are a class of ILs very often used in organic chemistry, as solvents and as precursors of N-heterocyclic carbene (NHC), very efficient ligand and organocatalyst. In fact, the deprotonation of the C2-H in between the two imidazolium nitrogen atoms leads to the formation of a singlet carbene, which can act as a base and/or nucleophile. This deprotonation is usually carried out using chemical bases or by cathodic reduction (Scheme 1). [2]



Scheme 1. Generation of NHC.

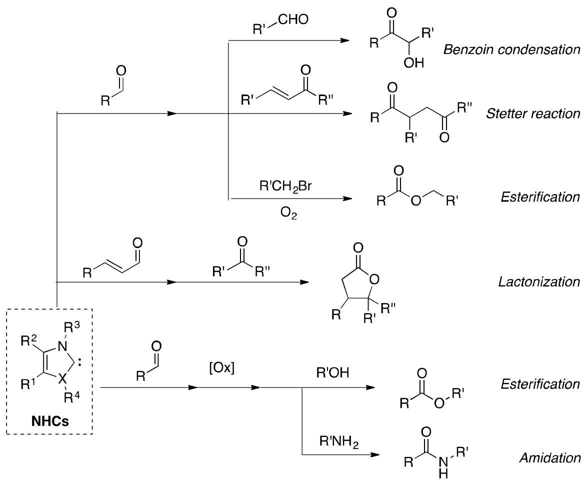
The advantages of the electrochemical deprotonation are the easiness of controlling the amount of reagent by simple control of the current, the "greeness" of the electron as reagent (non pollutant, generating no waste). Moreover, the ionic liquid can be used as both solvent-supporting electrolyte system and as reagent.

Moreover, the electrochemical methodology has also the advantage of being able to quantify the amount of NHC simply recording a cyclic voltammetry. In fact, the NHC obtained by cathodic reduction of the imidazolium cation ($BMIm^+$) can be oxidised at a potential near 0 V and its concentration is proportional to the peak current corresponding to this oxidation. Also ILs containing two imidazolium moieties can be easily deprotonated by cathodic reduction, yelding the corresponding mono- and dicarbenes (Scheme 2). [3] In all cases, NHCs can be used as efficient organocatalysts, involving mainly the umpolung process.



Scheme 2. Electrochemical generation of di-NHC.

Among the reactions thus carried out, we cite the benzoin condensation, the Stetter reaction, the oxidative esterification, the lactonization and the amidation of aldehydes (Scheme 3). [4]



Scheme 3. NHC-induced chemical transformations.

ILs can also be used in sensors. [5]

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New Organic Semiconductors for Electronics

The research is focused on the chemical synthesis, along with electrochemical characterization, of compounds with interest in the field of Organic Electronics. This somewhat generic term is used to indicate the vast field of science regarding the use of organic materials (either “small” molecules, oligomers or polymers) in electronic devices. Thiophene derivatives, especially in form of oligomers and polymers, surely fall in the class of the most studied (and used) organic semiconductor materials, probably because of their excellent charge transport properties and well-established synthetic procedures. There are countless applications of these materials in devices used as: OLEDs, Organic Photovoltaics, Sensors, OFET, Organic Photodetectors [1], and the number is continuously growing. Polythiophenes were the first and most studied thiophene derivatives, and some of them are still today viewed as reference materials, but they present some intrinsic disadvantages such as the absence of well-defined chemical structures and, thus, of reproducibility. Instead, for the abovementioned applications, high grade of purity and synthetic reproducibility are requested, in order to clearly address the synthesis of materials with precise and specific properties. These requisites are fulfilled by oligothiophene derivatives: in many cases they possess better characteristics (physical, optical, electronic and self-assembly properties, possibility to work in solution, ease of purification, low-cost synthetic procedures, and so on) over their polymeric counterparts. Oligothiophenes can also be viewed, especially in the research field, as model compounds for the study of structure-property relationships relatives to polythiophenes. Dipolar push-pull (i. e.: molecules that present donor (D) and acceptor (A) moieties) chromophores with highly polarizable π- electron systems possess properties that result from the existence of photoinduced intramolecular charge transfers at low energies. In particular, thiophene oligomers possess extended π-electron delocalization along the backbone and are good hole-transporting materials, and they can be synthesized with different Donor-Acceptor architectures (see Fig. 1) in order to fine tuning their optical and electrochemical properties [2-4].

Figure 1: Newly synthesized Oligothiophenes.

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Research activity on structural morphological and electrochemical materials characterization

The research activities on structural morphological and electrochemical materials characterization are described below:

Unconventional electrochemical systems for energy production and storage

The study consists of researching cathode and anode materials for lithium ion and lithium-ion batteries. Materials for this purpose are $LiMn_xFe_{(1-x)}PO_4$, Li_2S, core–shell $S–TiO_2$ cathode materials as well as amorphous nanometric carbon, as anode material. The materials are characterized structurally, [1-4] morphologically and electrochemically.

Morphological-structural investigations of electrode and non-electrode materials

The lithium intercalation mechanisms in the various crystalline structures of cathode materials are studied, following the variations of the crystallographic parameters during the process. In this way, more information on the intercalation mechanism can be obtained. For example, for primary cells the destruction of the host structure coincides with the end of the discharge. This research is carried out through the X-ray analysis of samples with various degrees of intercalation. In this research topic, electron microscopic analyzes are also carried out to observe the morphology of the cathodic powders and to determine the influence it has in the performance of the process. The surface area developed by these cathode materials is also very important and is measured with the technique based on the theory of Brunauer, Emmet and Teller (BET). The structural and morphological characterization activity does not end with the electrode materials but also extends to other materials used for other purposes such as, for example, the absorption and desorption of CO_2 [5] or biomaterials [6].

Electrowinning technique for indium recycling.

The increasing demand for indium as indium-tin-oxide (ITO) has led this metal to become a strategic material for the international commercial trade of green energy and audiovisual technologies. Many of these applications comprise flat display screens, optical sensor and optoelectronic systems, semiconductors and photovoltaic solar cells. Thus, an indium excessive demand and consumption for high-tech applications have made this metal to reach the top of critical materials classification. Since indium is considered a strategic material, a study for developing and optimizing a recovery process by electrowinning has been performed. The possibility of using electrolytic baths based on sulfates instead of chlorides has also been evaluated. Nowadays, chlorides are widely used because they generally present greater current efficiencies; however, the dangers of chlorine gas require expensive-sealed systems to avoid human health environmental issues. Therefore, studies to evaluate proper metal cathodes for indium electrowinning based on deposit morphologies, current efficiency and energy consumption have been performed using a fixed sulfate solution on stainless steel (SS) [7] and other different metal cathodes (Ni, Ti, Al and Cu) [8].

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Mass spectrometry for the analysis of complex matrices

Nowadays, mass spectrometry, coupled with chromatographic separation, is the most used technique for the analysis of complex matrices, as plant extracts, agri-food products, clinical samples, or chemical reaction mixtures, just to make some examples.

My most recent research activity combined my main interests for years:

- molecular electrochemistry of bioactive compounds, with mechanistic and synthetic purposes;
- natural antioxidants;
- mass spectrometry.

The electrochemical oxidation of caffeine and theophylline, methylxathines widespread in nature and in highly consumed products, and of interest from different points of view, from antioxidant properties and pharmaceutical applications to suitability as building blocks in organic synthesis, was carried out by controlled potential electrolysis, and the oxidation products were identified by mass spectrometry analysis after chromatographic separation. The research, carried out in collaboration with the LEOS-MS group, led to hypothesis of mechanisms useful to shed light on discussed antioxidant properties of such molecules, and to interesting product for synthetic applications [1, 2] (Figure 1).

An interesting review is placed in this contest, regarding the use of the smart material graphene oxide for the selective detection of natural methylxantines as caffeine and theophylline [3].

As another example, mass spectral analysis, combined with computational analysis, supported interesting results regarding the electro-synthesis of N-(cyclohexylcarbamoyl) acetamide [4].

Due to the interest towards natural antioxidants and the beneficial health effects due to diet antioxidants rich food and beverages, a novel, fast, selective and sensitive method for the analysis of phenolic compounds by HPLC-PDA-ESI-MS/MS was developed, validated, and applied to craft beers degassed, filtered and diluted, in collaboration with DICMA [5].

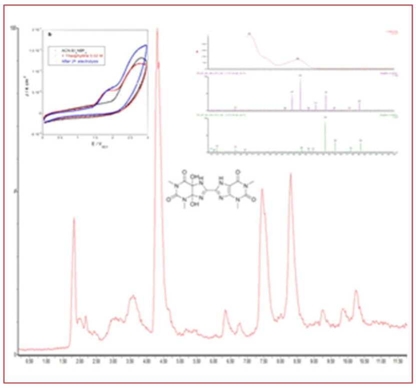

Figure 1. Main electro-oxidation products of theophylline by HPLC-PDA-ESI-MS/MS analysis

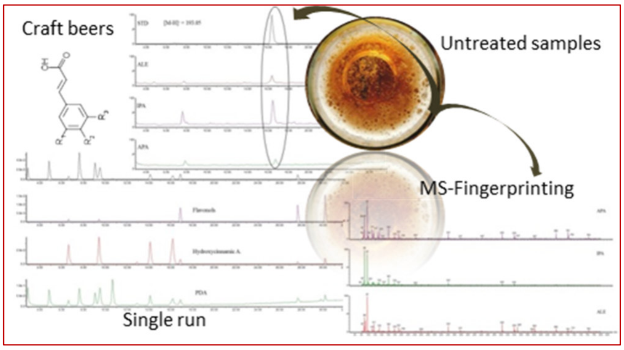

Figure 2. HPLC-PDA-ESI-MS/MS method for fast, selective and sensitive analysis of phenolic compounds in complex matrix.

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Thermal behavior study and assessment of thermal stability of different classes of materials

The thermal behavior study is a key step in the characterization of several classes of materials. In fact, the knowledge of these evidences is of paramount importance in the case of fire accidents, or if some materials were stored in places where they may reach very hot temperatures, especially during the summer. Thermal analysis techniques provide to investigate the change of some physical or chemical properties (i.e., mass and the heat flux for thermogravimetry and differential scanning calorimetry, respectively) of a material in the condensed phase.

In the period 2018-2020, my research activity has been focused on material science with particular reference to the thermal behavior study of different classes of materials, like: lead halide perovskites, mortars, geopolymers, organic-inorganic hybrids (OIHs), plastic waste, ionic liquids.

They represent a wide class of materials with characteristic properties remarkably different from one to another. In spite of this, for all of them we determined the temperature ranges for which they underwent physical or chemical processes (i.e., melting, crystallization, phase transition rather than dehydration or decomposition, respectively).

The thermal behavior of silica-based gel glasses or silica-based OIHs with either polyethylene glycol (PEG) and poly(ε-caprolactone) (PCL) as the organic component was studied with the view to find the most suitable temperatures for the thermal treatment to improve their properties [1,2]. Structural properties were also studied by X-ray diffraction analysis, while FTIR analysis showed that all these OIH materials belong to the first class due to the presence of hydrogen bonds between the –OH groups of the oxide and the ethereal oxygen atoms (H-bond acceptors) or terminal –OH of the PEG and PCL chains.

Pyrolysis seems a promising route for recycling of plastics from waste electrical and electronic equipment (WEEE). Thermal analysis experiments under inert atmosphere allowed us to study the thermal and catalytic pyrolysis of synthetic mixtures containing real waste plastics, representative of the most abundant polymers in small WEEE, even in the presence of two different zeolite-based catalysts containing high percentages of silica: HUSY and HZSM-5 [3,4].

The thermal analysis of metakaolin-based geopolymers incorporated in waste glass was studied. A comprehensive characterization was made using FTIR (to reveal the formation of bonds between the clay and the glass within the geopolymer matrix. Thermogravimetry showed that about 20% by mass of water was retained in all samples and released up to 500 K, and a lower amount was removed by dehydroxylation in the glass-rich samples due to the lower degree of reticulation (that means a lower number of hydroxyl groups underwent to condensation) [5].

Vaporization studies performed using effusion Knudsen and thermal analysis techniques have also been aimed at measuring the evaporation enthalpy and in the most favourable cases the absolute vapor pressure data for ILs, which are still scarce and uncertain, mostly limited to a few classes of stable compounds. In addition, though they are thermally stable compared to molecular solvents, they can start to decompose at the same temperatures where their vapor pressures become measurable. Two techniques based on molecular effusion under reduced pressure (under Knudsen regime) were considered. They both aimed at studying the thermal decomposition of tetramethylammonium lead iodide [6]. The heat capacity and thermodynamic functions of di-, tri- and tetramethylammonium lead iodide perovskites was also investigated in the range 289 - 473 K [7].

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Research Activities: Mathematics

Mathematics-Introduction

Several natural processes in physics, chemistry and in other applied sciences require the use of mathematical models. The realization of such models play an ever increasing role and today, more than ever, mathematics is the language of science. The study of differential models, evolutionary or stationary, continuous or discrete, deterministic or stochastic, contributed to the growth of many abstract disciplines as partial differential equations, differential geometry, numerical analysis, discrete geometry, harmonic analysis, graph and network theory and spectral analysis, just to mention a few. All these tools help to understand and predict the behavior of complex systems. We briefly expose some of the activities of the researchers in mathematics at our department and their interaction with applied sciences.

Discrete geometry, representation theory and harmonic analysis (Capparelli, Cerulli Irelli, Conti, Pepe,Vietri)

Discretization of a continuous model is of great help in computation, and this contributed to the development of the vast field of discrete mathematics; in geometry, it lead to graph theory and combinatorics. The research here focused on orthogonal polynomials, combinatorial aspects of Lie algebras and the interplay between representations of infinite dimensional algebras and integer partition theory. An important development is the idea of Vertex Operator Algebra by J. Lepowsky, I. Frenkel, A. Meurman, and by R. Borcherds, who received the Fields medal for related work in 1998. The study of algebraic varieties over finite fields found new applications to extremal combinatorics and extrema graphs. Graceful trees play a special role in many different situations in graph theory, also because a conjecture states that all trees are graceful. Progress is reported here in the study of graceful graphs and graceful trees. Finally, contributions have been made to the *problème des rencontres*, a well-known problem in enumerative combinatorics and in probability.
Representation theory is a unifying field of research because it plays a crucial role role not only in mathematics, but also in the physical sciences. Besides representations of infinite dimensional algebras, a special attention is devoted here to the representations of finite dimensional algebras and their naturally related geometric objects, i.e. quiver grassmannians and flag varieties. In particular, in the given period, a project about quiver Grassmannians was completed and a new project concerning the study of the orbit closures for symmetric quiver algebras has been initiated.
The basic idea of harmonic analysis is to decompose a functions space into a direct sum of eigenspaces, so that one could express a functions as a superposition of simpler eigenmodes. This has crucial applications in all applied sciences. The focus here is to move from the abelian situation to the non-commutative one, following the work of A. Connes; his program represents an important tool to describe, among other things, quantum systems and quantum gravity. Central topics and tools are $C^\star$ algebras and $C^\star$ dynamical systems. Progress was also made in the study of geometric and combinatorial group theory, following the approach by V. Jones, in turn inspired by Topological Quantum field Theory.

Evolution models, control theory, inverse problems. (Bruni, Carillo, Giacomelli, Lai, Leonori, Loreti, Petitta, Pitolli, Sforza, Vivaldi)

The evolution in time of a given system can be modelled by time dependent partial differential equations whose solutions represent different quantities related to the system. Using these differential models one could be interested in the observability and controllability of a system, in qualitative properties of the solutions (including singularities or finite energy properties or comparison principles), in scaling laws, or well−posedness of the problem.

Recently Fourier methods have been used in the study of alternating and variable controls for the wave equation and simultaneous observability and controllability of systems of strings and beams.
Octopus arms have attracted the interest in bio-inspired robotics, in particular, in the framework of soft manipulators so that mathematical control models for octopus arm are an interesting field in control theory.
Forward−backward parabolic equations are ill-posed and they develop singularities (e.g., Dirac measures). The description of temperature stratification in the ocean, some aggregation phenomena in biology, and Perona-Malik diffusion in image processing naturally lead to this kind of equations.
In the same way flux-saturating diffusion equations, which describe a saturation mechanism appearing at high gradients of the solution, exhibit formation of shocks (i.e. jump discontinuities).
Singular evolution boundary value problems (and their stationary counterpart) are involved in some problems of thermo-conductivity, in signal transmissions, and in the theory non-Newtonian pseudoplastic fluids. The singularity appears in nonlinear zero order terms which become infinite where the solution vanishes. Existence and uniqueness of finite energy solution are natural questions.
Some other theoretical questions about solutions of nonlinear evolution boundary value problem, like comparison principles, have a general interest, in particular if one has first order terms depending on the gradient of the solution in a superlinear way.
Inverse problem like Electroencephalography (EEG), Magnetoencephalography (MEG) are ill-posed and ill-conditioned problems and they require convenient numerical procedures in order to reduce significantly the dimension of the inverse problem thus reducing both memory usage and computation time.
Non-stationary signals analysis is often required in several applied fields, such as radar and micro-doppler systems, seismic or biomedical signals or gravitational waves. One can model, via an evolution law, the time-frequency distribution of non-stationary signals, defining computational methods for their decomposition into simple modes.
Materials with memory appear in viscoelaticity, in magneto-viscoelaticity or in rigid thermodynamics. They are materials whose mechanical and/or thermodynamical behaviour depends also on the past times. The contribution of the history of the material can be modelled via the introduction of an integral term in the evolution model. Various kernels are introduced to describe different behaviours and some wave-type problems with integral terms are considered from the observability and reachability point of view.

Nonlinear diffusion in composite materials, irregular structures, equilibrium states, graphs and networks (Amar, Andreucci, Camilli, Capitanelli, Cirillo, De Cicco, D'Ovidio, Giachetti, Lancia, Pezza, Zappale)

Processes of non linear diffusion can take place across heterogeneous or irregular structures as well as along graphs and networks.
Composite materials are characterized by the fact that they contains two or more constituents finely mixed according to a very small parameter. The heterogeneities are small compared with the global size of the body and two scales characterize the material, the microscopic one, describing the heterogeneities and the macroscopic one, describing the global behavior of the composite, which looks like a homogeneous material.
These materials exhibit in general a better behavior than the average of their constituents and for this reason they are widely used nowadays in industrial processes or in material science.

Let us just mention the example of the multifilamentary superconducting composites used in the manufacture of optical fibers or the example of polymers which are enhanced by highly conductive inclusions or perfect heat conductors.
From the mathematical point of view, diffusion throughout composite materials leads to study the asymptotic behavior of a PDE depending on a small parameter.
Moreover many biological processes as well problems of data trasmission or traffic management are controlled by complex interactions which evolve on irregular spatial domains and the Euclidean setting is only a first approximation to the complexity of the problem. Hence the increasing interest in the study of nonlinear differential models on networks, on ramified spaces and on graphs.
On the other hand a lot of natural phenomena take place across irregular and wild structures, tipically fractals, in which boundaries are "large", while bulk is "small" like for example organic molecules or metabolites in biological cells or brain tissue, particles in porous media, oxygen in human lungs, ions near rough electrodes or cellular membranes, gas in fractures.
Spatial heterogeneities can also either slow down or speed up particle motion giving rise to the so called *anomalous diffusion*. Namely, the sub–linear behavior of the mean square distance traveled by Brownian particles with respect to time is observed in cells due to macromolecules playing the role of large obstacles for the motion of smaller molecules.
Fractional equations, that are equations involving fractional operators in time and in space can model anomalous diffusions in the subdiffusive or superdiffusive case.
Integro-differential equations of fractional order are also used to model wave propagation in porous materials.
The previous PDE setting describing nonlinear heat and mass diffusion is naturally connected with minimization of suitable integral functionals in local and nonlocal framework.
Indeed many problems in applied sciences are formulated as equilibria and integral representations of energies are often needed in applied framework like elasticity, plasticity, fracture mechanics or micromagnetics.
Moreover extensions of well known theories like Anzellotti's pairing theory can be very useful in hyperbolic conservation laws and transport equations, as well as in problems involving the 1-Laplace operator. This operator is known to be closely related to the mean curvature operator and it enters in a variety of both practical and theoretical issues as for instance in image restoration and in torsion problems.

Partial differential equations in Geometry and Physics (Ianni, Pistoia, Provenzano, Savo)

The search for the optimal geometric configuration of a given system leads to a variational principle, and in that case the physical law is described by a partial differential equation, the Euler-Lagrange equation. This shows the deep interplay between mathematical physics, differential geometry and the theory of PDE's.
The research in this area mainly focused on nonlinear elliptic equations, nonlinear systems and geometric spectral theory.
When a gas of bosons at low densities is cooled to temperatures very close to absolute zero, a state of matter arises, the Bose - Einstein condensate (BEC). The Gross - Pitaevskii system consists of two coupled nonlinear Schrödinger equations, and is a mathematical model for the binary Bose - Einstein condensate for the unknown condensate wave functions. Progress has been made for phase separating solutions in general planar domains.
In astrophysics, Lane - Emden type equations model self-gravitating spheres of plasma, such as stars or self-consistent stellar systems; they are semilinear with a power focusing nonlinearity. The research mainly focused on the existence and the qualitative properties of

the solutions to these equations, in dependance of both the power p and the domain. The 2d case has been considered, addressing the following questions: uniqueness for the positive solution when the domain is convex, asymptotic behavior when the power p tends to infinity, Morse index estimates and multiplicity results.

Spectral Geometry investigates relationships between geometric structures of Riemannian manifolds and spectra of various elliptic operators. The research in this area put particular attention to: geometric upper bounds of Weyl type for the eigenvalues of the Neumann p-Laplacian and the Steklov problem, geometric estimates under Robin boundary conditions, asymptotic behavior of eigenvalues of the Steklov problem, ground state energy estimates for the magnetic Laplacian and Morse index estimates of self-shrinkers in terms of topology.

Thermal diffusion problems in composite media

The properties of composite materials have a wide spectrum of applications in industrial processes, and thus their study plays a crucial role in the framework of material sciences. Composite materials are often modeled by means of an underlying structure containing a large number of microstructures disposed in a periodic array and are grounded on the interplay of phenomena which take place at different space and time scales. Moreover, many physical situations display also the presence of interfaces, whose behaviour has an active role in the description of the phenomenon. A well known approach to this kind of problems is based on the homogenization techniques which are applied in order to simplify such schemes and make them amenable to numerical approximations. In the literature, various homogenization techniques have been proposed. A recent approach, due to Cioranescu-Damlamian-Griso, is based on the introduction of the so-called periodic unfolding operator. We have applied this technique to the study of models describing heat diffusion in composites involving materials which differ in structure and composition, but displaying similar behaviour.

More in details, we focused on the behaviour of polymers which are enhanced by highly conductive inclusions or perfect heat conductors, i.e. inclusions having infinite thermal conductivity (this last assumption being motivated by the fact that, in many applications, the heat conductivity of the inclusions is much larger than the one of the hosting medium). In some of these cases, things are made even more complicated, since the nanoparticle fillers have their own film coating separating them from the surrounding polymer. This surface enhancement of the nanoparticles is useful, for example, to improve their dispersion and also the electrical properties of the composites. Such reinforced polymers give rise to efficient materials for encapsulation of electronic devices.

We focused our interest on the rigorous study of these composites which deserve very interesting mathematical aspects. Indeed, the presence of such inclusions implies that, at the separating interface, non-standard or nonlocal interface conditions are assigned.

More precisely, in some of these models the description of the thermal diffusion along the interfaces is modeled by means of the Laplace-Beltrami operator. Other suitable models describing the behaviour of such physical materials lead to the so-called equivalued surface boundary value problems, where the thermal diffusion on the interfaces are governed by the so-called non-local flux conditions. It is worthwhile noting that non-local boundary conditions have a wide area of possible applications ranging from heat diffusion to electric conduction, to petroleum exploitation, to wave equations or to the elastic behaviour of perforated materials.

We also studied models, representing the equilibrium for the heat conduction in composite materials as well as boundary layer phenomena for viscous or non-Newtonian fluids, or even the enzymatic kinetics, in which the presence of active interfaces is coupled with nonlinear source terms of singular lower order type.

We stress the fact that the common feature of all the previous problems is the presence of interfaces between the different phases, whose physical behaviour is relevant to determine the effective properties of the media from the macroscopic point of view.

Another important aspect of our research is a typical mathematical approach connected with existence and uniqueness problems. Indeed, the models previously considered are mathematically described by means of systems of PDEs involving elliptic, parabolic, pseudo-parabolic or abstract parabolic equations and, due to the presence of active interfaces, also tangential operators could appear. Moreover, in several situation, also the underlying geometrical structure plays a crucial role. In many cases, these PDEs systems are anything but standard and they need a delicate investigation in order to assure that they are well-posed.

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Nonlinear diffusion on graphs and manifolds

Asymptotic estimates for the p-Laplacian on graphs.
In [1] we apply some ideas coming from the theory of continuous Partial Differential Equations, namely the methods relying on local sup estimates, to the case of degenerate diffusion on graphs. The graph G is assumed to be simple, unidirected, infinite, connected, with weight w and V is the set of its vertices. The relation $x \sim y$ holds if and only if x and y are connected by an edge. We look at the problem

$$\begin{aligned} \frac{\partial u}{\partial t}(x,t) &= \Delta_p u(x,t)\,, \qquad && x \in G\,, t>0\,,\\ u(x,0) &= u_0(x) \geq 0\,, && x \in G\,. \end{aligned}$$

Here $p > 2$, $d_w(x) = \sum_{y\sim x} w(x,y) < +\infty$,

$$\Delta_p u(x) = \frac{1}{d_w(x)} \sum_{y\in V} |u(x)-u(y)|^{p-2}(u(x)-u(y))w(x,y)\,.$$

We assume a convenient version of the Faber-Krahn inequality, stated of course in terms of finite differences. We prove an a priori estimate connecting the supremum of a solution u to the measure of its level sets, which we then use to prove existence and uniqueness of a global in time solution for every integrable initial data. We provide both sup estimates of u and integral estimates of the difference gradient.
In graphs, the property of finite speed of propagation for degenerate equations like ours is known to fail, due to the discrete character of the topology. However we prove a result bounding the effective speed of mass diffusion, which we use also to prove the optimality of the mentioned sup estimate.
Finally, we provide estimates for solutions corresponding to slowly decaying initial data u_0, that is data which are not integrable on V, though some power u_0^q, $q > 1$, is integrable.

Extinction of non-negative solutions to fast diffusion equations on manifolds.
In [2] we considered the Cauchy problem

$$\begin{aligned} \rho(x)\frac{\partial u}{\partial t} &= \operatorname{div}(u^{m-1}|\nabla u|^{p-2}\nabla u)\,, \qquad && \text{in } M\times(0,T),\\ u(x,0) &= u_0(x)\,, && x\in M\,, \end{aligned}$$

where M is a non-compact Riemannian manifold of topological dimension N, satisfying a p-hyperbolicity assumption, with Riemannian measure μ; u_0 is a non-negative integrable initial data. The positive weight function ρ is radially decreasing (with respect to the distance d from a fixed point $x_0 \in M$). Let $B(d(x))$ be the ball of radius $d(x)$ centered at x_0. We look at the fast diffusion case, that is we assume

$$p+m-3<0\,, \qquad N>p>1\,.$$

It is well known that under similar assumptions in the Euclidean case $M = \boldsymbol{R}^N$ and for $\rho(x) = (1+|x|)^{-\ell}$, the solutions vanish in a finite time if

$$\ell > \frac{\beta}{p+m-2}\,, \qquad \beta = N(p+m-3)+p\,.$$

Here we give a criterion for extinction in a finite time relying on the interplay between the Riemannian metric and the nonlinearities appearing in the equation. The metric appears in fact via the isoperimetric functions

$$\omega(s) = \frac{s^{\frac{N-1}{N}}}{h(s)}\,, \quad h(v) \leq |\partial U|_{N-1}\,, \quad \mu(U) = v\,.$$

The result follows from a weighted embedding inequality of Minerbe type, and guarantees extinction if, for $p^* = \frac{Np}{N-p}$,

$$\int_M \{\rho(x)\omega(\mu(B(d(x))))^{\delta}\}^{\frac{p^*}{p^*-\delta}} \mathrm{d}\,\mu < +\infty\,,$$

and $\delta \in (p, p^*)$ if $\beta \leq 0$, $\delta \in (p, (p+m-2)/p) < p^*$ if $\beta > 0$.

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Authors
D. Andreucci

Time-frequency analysis of non-stationary multicomponent signals

The research activity focused on modeling the time-frequency distribution of non-stationary signals, and on defining computational methods for their decomposition into simple modes. To this aim time-frequency analysis, numerical methods and approximation theory tools have been employed and developed.

Motivation Non-stationary signals analysis is required in several application fields, such as radar and micro-doppler systems, seismic or biomedical signals, gravitational waves, audio and human speech signals. Non-stationary signals are the superposition of amplitude and frequency modulated (AM-FM) modes. Crucial tasks in their analysis are components separation and instantaneous frequencies (IFs) estimation, i.e., the derivatives of the time-dependent modes phase. Reassignment makes sparser signal time-frequency distribution (TFD) and allows to better localize signal modes. Unfortunately, TFDs suffer from the presence of misleading cross terms caused by the interference of non-separable modes, making modes separation not accurate.

Main results A time-frequency (TF) evolution law (pde) for signal spectrogram has been written, and the definition of modes separability has been relaxed [1]. The pde explicitly depends on IF first derivative and the logarithmic derivative of modes amplitude; in addition, it allows us to characterize points that are less influenced by cross terms, i.e. those satisfying the weak separability condition. Based on these theoretical results, the following computational methods have been developed.

Modes counting: signal TFD is modeled as a non-stationary process switching from locally separable to non-separable modes. Kolmogorov complexity is used to model the information conveyed by TFD, and signal complexity is evaluated by run-length encoding the binary TFD. Complexity temporal variations allow for signal modes counting [2] (Fig. 1: 1^{st} row).

Spectrogram reassignment: spectrogram integral (wrt frequency) is a multicomponent signal with specific IFs. A numerical procedure has been defined to disentangle frequencies and to recover the missing information in the interference region. Modes weak separability is used for improving reassignment in the interference region without assumptions on IF kind, but subject to the absence of amplitude modulation. Iterative methods that converge to modes IFs have been defined for pointwise reassignment [1,3]. An acceleration scheme has been developed to increase convergence rate, while limiting conditions on the initial guess. The reallocation method is fast and localizes signal modes independently of interference effects (Fig. 1: 2^{nd} row).

IFs separation: TFD and Radon transform are jointly used for unsupervised modes separation in noisy conditions [4]. The method takes advantage of the ability of the Radon transform in separating overlapping modes (Fig. 1: 3^{rd} row). It consists of a blind segmentation in Radon domain through a near-to-optimal threshold. Transform inversion of each detected region allows for modes IF separation in the TF domain (Fig. 1: last row).

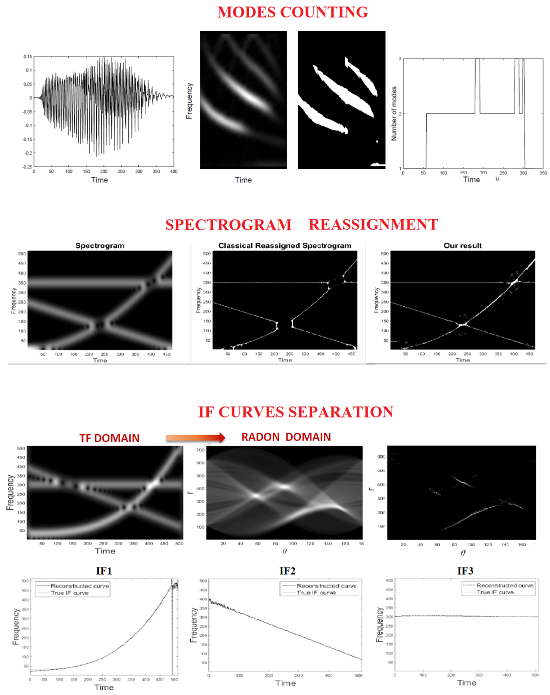

Figure 1: 1^{st} *row:* 3-modes signal, signal TFD, its binarization, estimated no. of modes. 2^{nd} *row:* 3-modes signal TFD, amplitude-based reassignment, proposed reassignment. 3^{rd} *row:* TFD of a 3-modes signal, Radon transform, its segmentation. 4^{th} *row:* estimated IFs.

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V. Bruni, M. Tartaglione, D. Vitulano

Mathematical models for interacting systems

Aim of this research line was the study of some Partial Differential Equations (PDE) arising as models of biological processes and other systems (such as e.g., crowds, animal groups, cell colonies) involving individuals who possess some decisional abilities. Indeed complex systems have attracted interest in various fields, from Sociology to Economyy and Biology since they pose new and stimulating scientific challenges with respect to more traditional systems:
"Today, most of science is biology" (Reed, "Mathematical biology is good for mathematics", Notices of AMS, 62, 2015)
and also in Mathematics biological applications are becoming the main driving force of innovation.
Many biological processes are controlled by complex interactions which are not well described by a classical setting even in the case of Euclidean geometry and therefore require differential models with a more flexible structure. In addition often such processes evolve on irregular spatial domains and the Euclidean setting is only a first approximation to the complexity of the problem. Hence the increasing interest in the study of nonlinear differential models on networks, on ramified spaces and involving nonlocal terms.
In this project we concentrated on differential problems as outlined above with the following objectives:

(i) A correct mathematical formulation of interacting models with special attention to

- PDE defined on networks and other irregular geometric structures
- PDE with nonlocal terms

(i) The extension to the new setting of classical functional analysis techniques in order to study the well posed-ness of the previous problems.

(iii) The development of numerical methods and algorithms for the validation of the theoretical results.

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Analysis on irregular structures

Our research focuses on the study of Partial Differential Equations arising as models of diffusion processes on irregular structures: domains with non-smooth boundaries, fractal boundaries and fractal layers. Irregular structures may occur as (part of) boundaries of Euclidean domains in Boundary Value Problems (BVPs). As layers, irregular structures may occur at the common boundary of two adjacent Euclidean domains. Analytically, on such layers, first, second or fractional order transmission conditions are satisfied. These conditions involve at the same time traces of functions from classical Sobolev spaces, normal derivatives on the layer and intrinsic operators which are technically delicate in the fractal case. To deal with such problems, one has to develop new analytical concepts and tools; new frames must be set, hopefully encompassing basic features of Riemannian metrics, but having a range wide enough to fit the new fractal phenomena.

Analysis on regular structures has been one of the central areas of mathematical research in the 20th century. In the last decades of the 20th century, there was an explosion of interest in fractal geometry motivated, on the one hand, by the advances of mathematicians who used Hausdorff measures to extend Euclidean geometry beyond smooth manifolds up to fractal objects, and, on the other hand, by the insight of mathematicians such as Mandelbrot who showed the rich potential of fractal geometry to provide suitable models for problems encountered in physics, and in natural and social sciences.

A theory of analysis on fractals is recent. This analytic theory exhibits striking differences from its smooth Riemannian counterpart. For instance, notions of dimension arising in connection with Weyl-type asymptotics and heat kernel estimates do not always coincide with corresponding geometric notions of dimension such as the Hausdorff dimension in either the ambient (extrinsic) Euclidean metric or the intrinsic metric. On the other side, the study of phenomena in which classical boundary value problems merge with the theory of fractal sets and fractal operators – as they occur, for example, when modeling diffusion phenomena across fractal layers of Koch type – is emerging.

Some first examples in the literature of the study of problems in which classical BVPs merge with the theory of fractal sets and fractal operators are due to our group.

Our project focuses on both theoretical and numerical study of (possibly nonlocal) BVPs in domains with fractal boundaries and/or interfaces.

In particular, we mention results regarding the periodic homogenization of the stationary heat equation in a domain with two connected components, separated by an oscillating interface defined on pre-fractal Koch type curves [1].

Moreover, we mention the study of obstacle problems involving p-Laplace-type operators in non-convex polygons like pre-fractal Koch Islands [2]. We established regularity results in terms of weighted Sobolev spaces and, as application, we obtained estimates for the FEM approximation for obstacle problems in pre-fractal Koch Islands.

In the framework of fractional diffusion, in [3] we studied parabolic diffusion problems for the regional fractional Laplacian with Robin-type boundary conditions in irregular domains, in particular of fractal and pre-fractal type. We proved existence and uniqueness results for the "classical" solution as well as regularity properties of the associated semigroup. Moreover, we studied the asymptotic behavior of the pre-fractal solutions, proving that they converge in a suitable weak sense to the fractal one.

Moreover, in [4] we studied the regularity of the weak solution of a heat equation coupled with nonlocal (dynamical) Venttsel' boundary conditions in piecewise smooth domains. In particular, we proved that such weak solution belongs to a suitable anisotropic weighted Sobolev space. We point out that regularity results of this type play a crucial role when considering the numerical approximation of problems in pre-fractal domains.

As many phenomena in physics and in nature can be modeled by fractals, the development of mathematical theories with the construction of new tools based on "fractal" concepts and techniques should help us in better understanding such phenomena. For example, it is shown experimentally that irregular morphology of the interface significantly speeds up heat transfer. This result suggests that irregular or fractal shapes can be used to increase heat removal from pulsed heat sources in electronics and microelectronic devices. Moreover, diffusion of medical sprays and oxygen transport to/across alveolar membranes in the human lungs are transport phenomena which occur across irregular layers well modeled by fractal curves and surfaces. Mathematical analysis of these problems is essential to confirm (or disprove) theoretical models based on experimental data.

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R. Capitanelli, S. Creo, S. Fragapane, M.R. Lancia, M.A. Vivaldi

Algebraic and combinatorial aspects of Lie algebras, orthogonal polynomials, hyperbolic polynomials

The research described below was carried out in the period under consideration and was partially supported by three grants of Ateneo-Sapienza for the years 2018, 2019, 2020. Described below in particular is that part of the research concerned with algebraic and combinatorial aspects of Lie algebras, orthogonal polynomials, hyperbolic polynomials.

1. The interaction between integer partition theory and the representation theory of certain infinite dimensional Lie algebras started from certain observations by J. Lepowsky and S. Milne of Yale who in 1978 found a connection between Rogers-Ramanujan identities and level 3 representation of the infinite dimensionale affine Lie algebra $\mathfrak{sl}(2, C)^{\sim}$. This gave rise to spectacular developments among which is the idea of Vertex Operator Algebra (VOA) by J. Lepowsky, I. Frenkel, A. Meurman, and by R. Borcherds, who received the Fields medal for related work in 1998. In collaboration with A. Meurman (U. Lund, Svezia) and M. Primc (U. Zagabria, Croazia) Capparelli proposed a number of new interesting combinatorial identities of the Rogers-Ramanujan type.

2. In earlier work by S. Capparelli the Bezoutian matrix was computed of a class of monic polynomials with integer coefficients. It was found that the Newton's symmetric functions for these polynomials satisfy certain very simple relations. In [3] the point of view was reversed and we determined four families of polynomials starting from given symmetric functions. Two of the families coincide with ones already known, two others were unknown.

3. According to a classical result of Kronecker's any algebraic integer which lies with its conjugates in the interval $[-2, 2]$ must be of the form $x = 2\cos\frac{2k\pi}{m}$. The corresponding polynomials are called *Kronecker polynomials*. If the interval has length less than 4 it can contain only a finite number of sets of conjugate algebraic integers, while any real interval of length greater than 4 contains an infinite number of them. The problem remains unsolved for intervals of length exactly 4. In the sixties, R.Robinson from Berkeley, classified all irreducible polynomials with integer coefficients having only real roots, such that the difference between the largest and the smallest root, (the *span*), is less than 4, for degrees up to and including 8. In recent years, S. Capparelli and collaborators extended Robinson's classification up to degree 14, moreover a list up to degree 17 was obtained and conjectured to be complete. In collaboration with A. Del Fra and A. Vietri we introduced a basis formed essentially by Chebyshev polynomials. With this basis we were able to easily obtain many of the 158 previously known polynomials. At the same time. the fact that no new polynomial has been found seem to give some credit to a conjecture that there may be no such polynomials with degree higher than 18. This has been published in [1].

4. The *problème des rencontres* is one of the classical problems in enumerative combinatorics and in probability. In [4] we extend the *problème des rencontres* to *generalized permutations* namely, certain particular bijective functions. More precisely, given an n-set X and two m-sets U and V, such that X, U and V are pairwise disjoint, we consider a bijection of the set $X \cup U$. In collaboration with V. Pepe e A. Del Fra we found a connection between derangements and generalized Laguerre polynomials,[2].

Some of these results have been presented in conferences such as Vertex Algebra and related topics, Zagreb 2018 (invited speaker), Combinatorics 2018, Arco (Trento).

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S. Capparelli, V. Pepe, A. Vietri

Recent advances in linear and non linear problems arising in investigating soliton theory and new materials properties: Bäcklund transformations & material with memory

The study presented can be summarised in two different research lines:

- Bäcklund transformations in investigating nonlinear partial and ordinary differential equations;
- materials with memory: viscoelaticity, magneto-viscoelaticity and rigid thermodynamics with memory.

On the first line, ref.s [1,2,3,5,6,8,10]. Bäcklund transformations represent a very powerful tool to investigate nonlinear evolution equations which admit so called *soliton solutions*. The long lasting research project, is is concerned about various applications of Bäcklund transformations. The results obtained are concerned about symmetry and structural properties as well as links connecting nonlinear evolution equations in the case of operator *soliton equations* [1,2, 8]. Specifically, in such references, the unknown is an operator on a Banach space. Notably, new connections are revealed. As a special case, of interest in applications, matrix solutions are constructed in [10]. A comparison between the classical case of a real valued unknown and the case of an operator on a Banach space is analysed in [6] where differences as well as analogies between the two different cases are considered. Bäcklund transformations are the key too also in investigating nonlinear ordinary differential equations. In [3] new solutions of the Ermakov-Pinney and Emden-Fowler equations are obtained via Bäcklund transformations. In [5] the Gross-Pitaevskii equation is studied: Bäcklund transformations and admitted solutions are studied. A nonlinear problem arising in nonlinear thermodynamics is investigated in [11].

To the second research line are the results in ref.s [4, 7, 9, 12, 13]. *Materials with memory* are termed those materials whose mechanical and/or thermodynamical behaviour depends on time not only on the present but also on the past times. Then, the contribution of the physically admissible history is modelled via the introduction of an integral term. The model has a wide applicability and various kernels are introduced to describe different behaviours. Specifically, in [4] a three-dimensional singular kernel problem in viscoelasticity is investigated. A further generalisation in which weaker regularity conditions are imposed on the relaxation function is investigated in [9] aiming to describe further viscoelastic materials. In [7] the case of an unbounded relaxation function in a rigid heat conductor with memory is studied. A magneto-elasticity problem on a disk is treated in [12]. An overview on thermodynamically admissible viscoelasticity models is provided in [13].

Finally, ref.s [14, 15, 16] represent introductions to Special Issues of journals devoted to collections of articles which were presented in conferences co-organised by S. Carillo.

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Geometric Methods in Representation Theory of Finite Dimensional Associative Algebras

Representation theory is a cross-disciplinary branch of pure mathematics and, as such, closely linked to many other fields in mathematics and science. Its scope is unusually wide. In chemistry, for example, representation theory is used in the investigation of the symmetries of molecules; in physics, quantum mechanics is a classic field of application. Other examples of applications in physics and related fields include integrable grid models, elementary particle theory, random matrix theory, string theory, and quantum computing. Among the many branches of mathematics in which representation theory plays an important role are algebraic geometry, topology, number theory, and differential geometry.

The research in this field at SBAI concerns the study of representation theory of finite dimensional algebras and of the geometry of naturally related algebraic varieties, e.g. quiver Grassmannians and orbit closures. Let A be a finite dimensional algebra. Up to technicalities, such an algebra is isomorphic to the path algebra of a finite quiver Q (i.e. an oriented graph) modulo an ideal generated by admissible linear combinations of paths. The quiver Q has finitely many vertices Q_0 and a module M for A is just a Q_0–graded vector space where the algebra A acts linearly. It is sometimes interesting to consider the situation where Q is endowed with an orientation-reverising automorphism σ inducing a self-duality on the category of its representations. In this case (Q, σ) is called a symmetric quiver, and the corresponding algebra $A = KQ/I$ is called an algebra with self-duality.

The research was focused on the following aspects:

1. Finish the project about quiver Grassmannians;
2. Connections between symmetric quiver algebras and 2-nilpotent Borel orbits for the orthogonal and the symplectic group;
3. Start a new project concerning the study of the orbit closures for symmetric quiver algebras;
4. Complete the study of linear degeneration of flag varieties.

We now give a brief description of the four objectives above:

- in collaboration with F. Esposito (Padova), H. Franzen (Bochum) and M. Reineke (Bochum) we have finalized the project concerning cellular decomposition of quiver Grassmannians and we have published the corresponding paper in Advances of Mathematics.
- In collaboration with M. Boos (Bochum) and F. Esposito (Padova) we have found a connection between 2-nilpotent Borel orbits for the orthogonal and the symplectic group and the representation theory of an algebra with self-duality of finite representation type.
- Motivated by the connection with Lie theory, in collaboration with M. Boos (Bochum) we have started the study of orbit closures for symmetric quivers.
- In collaboration with F. Esposito (Padova), E. Feigin (Moscow), G. Fourier (Aachen) and M. Reineke (Bochum) we have finished the study of linear degeneration of complete flag varieties and extended to the case of partial flags.

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Fluxes through heterogeneous materials

Spatial heterogeneities can either slow down or speed up particle motion: *anomalous diffusion*, namely, the sub–linear behavior of the mean square distance traveled by Brownian particles with respect to time is observed in cells and explained as due to macromolecules playing the role of large obstacles for the motion of smaller molecules. On the other side, in granular system it has been observed that obstacles can accelerate the dynamics, since a suitably placed barrier can improve out–coming flows by reducing the clogging at the exit. A similar behavior is shown by pedestrians in case of fast egress. This is a sort of inverse *Braess' paradox*, which states that if a supplementary link is added to a road network, it can happen that cars take longer to cross the network.

We investigated these phenomena in the framework of very simple models in order to capture their basic features without being thrown off by the countable number of possible explanations which come out in the study of complicated models.

In papers [12–15] we studied the effect of the barriers on the typical time that a particle needs to cross 1D and 2D strips for different simple dynamics, such as *simple symmetric random walk* and *linear Boltzmann dynamics*. A thorough study of the residence time properties as a function of the details of the dynamics and the geometry of the obstacles has been provided by using both Monte Carlo simulations and analytic tools. In particular, in the 1D case, we were able to set–up an exact computation of the residence time, which is also very useful to check the reliability of the simulations. It has been shown that the residence time is not monotonic with respect to size and position of the obstacles. In some cases, it is even shorter than the one measured for the empty strip, but displacing the obstacle along the strip can result either in an increase or decrease of the residence time. This complex behavior, although not intuitive, was explained as the result of the competition between two opposite effects: i) the time spent by particles in the channels flanking the obstacle is smaller than the total time spent in the central part (the region containing the obstacle) of the strip in the empty case; ii) the time spent by the particles in the regions on the left and on the right of the obstacle is larger with respect to the empty case.

Problems strictly related to this research line have been attacked in [1] and [11], where we have, respectively, used homogenization techniques to find upscaled equations for particles diffusing through a line of obstacle in presence of a non–linear drift and, starting from a microscopic lattice model, we derived in the hydrodynamic limit both the Fick and the Fokker–Planck diffusion equations by introducing site or edge heterogeneities. In [11] we have also shown how uphill currents can emerge when regions with different diffusion rules are in contact. Related results were also obtained in [8] in the framework of the Zero range Process. We also mention [7] where, in a 1D quantum set–up, we investigated the effect of periodic barriers on the particle flux and we shown that its computation can be reduced to the study of a suitable one dimensional stochastic process.

By using different geometries and elementary dynamics, we have also studied in [2,3,6] interaction between different particle species undergoing different dynamics. Application to pedestrian modelling have been exploited, focussing, on the problem of lane formation and blind egress. A three state spin system, the Blume–Capel model, has been used in [10] to study domain morphology under evaporation.

Finally, in [5] we modelled the presence of a membrane which is activated by passing particles in the framework of a 2D billiard model. We describe a transition between a homogeneous and an accumulated state by means of painstaking Monte Carlo simulations. We could also derive an analytic theory based on ergodicity assumptions.

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Operator algebras, Noncommutative Geometry and Quantum Field Theory

Research in the period 2018-2020 has been mostly focused on the following general topics:

- Noncommutative harmonic analysis;
- Symmetries of certain Cuntz-Pimsner algebras;
- Geometric/combinatorial group theory;
- Theory of superselection sectors;
- Applications of methods from category theory to noncommutative geometry.

The outcome of these studies has been collected in 11 articles that have been published in the period 2018-2020, plus other 7 that appeared in print in 2021.

More in detail, the first item (and actually the first three in the list) finds its place in the general area of *Operator Algebras* and deals with the general analysis of the structure of twisted crossed products associated to C^*-dynamical systems, and especially it is concerned with the uniform convergence of C^*-algebra-valued Fourier series in the very general setting of discrete groups, asymptotic invariance properties, (semigroups of) completely positive maps, completely bounded multipliers, etc.
The second item includes the study of several properties of the automorphism group and endomorphism semigroup of a natural class of C^*-algebras, with very challenging connections with the theory of semisimple Lie groups but also dynamical systems on Cantor sets and discrete mathematics/combinatorics. This study has been further divided into two parallel lines of research, one more abstract (e.g. the study of the general structure of the automorphism group), and one more concrete (i.e. the explicit construction of new classes of automorphisms). In the special case of the Cuntz algebras, it has been also studied in detail the structure of the endomorphisms associated to unitary solutions of the quantum Yang-Baxter equation (these are related to the braiding of suitable categories of representations of quantum groups and related objects).
The third item follows a new line of research initiated by V. Jones (Field Medalist 1990) and inspired by Topological Quantum Field Theory and specifically refers to the construction of certain unitary representations of the Thompson's groups (certain interesting subgroups of the homeomorphisms of the unit interval $[0,1]$, or the circle, or the Cantor set) in terms of suitable evaluations of graph and knot/link invariants; matrix coefficients of these representations are then related to analytic and algebraic properties of these fascinating but complicated groups.
Roughly, noncommutative geometry (in the sense of A. Connes, Field Medalist 1982) is a replacement of differential geometry in the noncommutative setting, and provides powerful tools for a rigorous mathematical description of quantum systems with nontrivial geometric content, most notably quantum gravity where one has to merge quantum field theory (QFT) with general relativity. As abstract C^*-algebras describe noncommutative topological spaces, spectral triples then describe spaces with a differential structure (which allows to deal with volume forms, connections, spin structure, etc.).
The fourth item is concerned with a way to use certain familiar objects in noncommutative geometry (i.e., Kasparov KK-theory) in order to describe the superselection structure of the scaling limit theory (the theory describing the short distance limit) of a given QFT directly in terms of the theory at scale one. The resulting objects are kind of (localized) asymptotic morphisms in the sense of Connes-Higson E-theory, i.e. behave more and more as genuine endomorphisms when the scale parameter $\lambda \to 0$. After a general analysis, most of the subsequent work has been devoted to study these objects in a concrete but important example, namely the so-called Schwinger model (QED in $D = 1 + 1$), for which some charges appear in the scaling limit that are not present at the ambient scale (confinement). In this setting it becomes quite important to understand the modular structure of Weyl algebras, especially a detailed analysis of the relation between the Tomita operators associated to bounded regions for the massive and massless scalar free theories, respectively.
Finally, the last item is very much in the same spirit as the previous one, but much more in depth as far as category theory is involved, in a way that climbs somewhat nontrivially the ladder of (involutive, C^*) n-categories. The goal of a related project is to provide a sound formulation of (categorical) noncommutative Gelfand duality, beyond the Dauns-Hofmann theorem, and based on the notion of spaceoid (a horizontal categorification of the concept of topological space).

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Some extensions of Anzellotti's pairing theory

In a seminal paper, Anzellotti in 1983 introduced a pairing $(\mathbf{A}(x), Du)$ between weakly differentiable vector fields $\mathbf{A}(x)$ and the measure derivative Du of functions $u \in BV$ of bounded variation. This pairing is an abstract mathematical tool very useful in many context and in its full generality has been revealed very fundamental in several applications.

Let us describe in more detail the functional setting of the problem. Let $\mathcal{DM}^\infty$ denote the class of bounded divergence measure vector fields $\mathbf{A}\colon \mathbb{R}^N \to \mathbb{R}^N$, i.e. the vector fields such that $\mathbf{A} \in L^\infty$ and the distributional derivative $\mathrm{Div}\mathbf{A}$ is a finite Radon measure. If $\mathbf{A} \in \mathcal{DM}^\infty$ and u is a function of bounded variation with precise representative u^*, then the distribution $(\mathbf{A}, Du)$, defined for every test function $\varphi \in C_c^\infty(\mathbb{R}^N)$ by

$$(\mathbf{A}, Du)\varphi := -\int_{\mathbb{R}^N} u^*\varphi \, d\mathrm{Div}\mathbf{A} - \int_{\mathbb{R}^N} u\, \mathbf{A} \cdot \nabla\varphi \, dx, \quad (1)$$

is a Radon measure in $\mathbb{R}^N$, absolutely continuous with respect to $|Du|$. This fact has been proved by Anzellotti for several combinations of $\mathbf{A}$ and u (for instance $\mathrm{Div}\mathbf{A} \in L^1$ or u a BV continuous function), excluding the general case of $\mathbf{A} \in \mathcal{DM}^\infty$ and $u \in BV$. Indeed, at that time, it was not clear how the discontinuities of u interact with the discontinuities of the vector field $\mathbf{A}$. The pairing (**??**) has been defined in the general setting by Chen–Frid, by characterizing the absolutely continuous part of the measure $(\mathbf{A}, Du)$ as the usual scalar product $\mathbf{A} \cdot \nabla u$. Nevertheless, they have not characterized the singular part of the measure, and, as far as we know, this problem has remained unsolved, at least in this general setting.

Our first aim in the paper [1] is to characterize the measure $(\mathbf{A}, Du)$ in the general case $\mathbf{A} \in \mathcal{DM}^\infty$ and $u \in BV$. We give a precise description of the jump part $(\mathbf{A}, Du)^j$ of the measure $(\mathbf{A}, Du)$ in terms of the trace of u and the normal trace of $\mathbf{A}$ and we are able to give a representation formula for the Cantor part $(\mathbf{A}, Du)^c$ of the pairing measure.

Among other applications that will be mentioned below, this theory can be used to extend the validity of the Gauss–Green formula to such vector fields and to non smooth domains. As a means of comparison, there are mainly two kinds of generalizations of the Gauss–Green formula. On one hand, one may consider weakly differentiable vector fields but fairly regular. On the other hand, De Giorgi and Federer consider fairly regular vector fields and sets of finite perimeter. Other generalizations deal with weakly differentiable vector fields and non-smooth domains. In the second part of the paper [1] we prove a Gauss–Green formula valid for both weakly differentiable vector fields and sets of finite perimeter. This unifying result is obtained by revisiting Anzellotti's pairing theory in the general case of divergence measure vector fields and BV functions. The core of the work is the characterization of the normal traces of these vector fields and the analysis of the singular part of the pairing measure. This will allow us to establish some nice formulas (coarea, chain rule, Leibnitz rule) for the pairing and, eventually, to prove our general Gauss–Green formula.

In the paper [2] we introduce a nonlinear version of the notion of Anzellotti's pairing between divergence–measure vector fields and functions of bounded variation, motivated by possible applications to evolutionary quasilinear problems. Our aim is to extend the pairing theory from the product $u\mathbf{A}(\mathbf{x})$ to the mixed case $\mathbf{B}(x, u)$. Our main assumptions on $\mathbf{B}$ are that $\mathbf{B}(\cdot, w) \in \mathcal{DM}$ for every $w \in \mathbb{R}$ and $\mathbf{B}(x, \cdot)$ is of class C^1. We prove that the nonlinear pairing $\mu := (\partial_w \mathbf{B}(\cdot, u), Du)$ is again a Radon measure, absolutely continuous with respect to $|Du|$. This formula generalizes the nonautonomous chain rule for BV vector fields. Notice that, when $\mathbf{B}(x, w) = w\,\mathbf{A}(x)$, then $\mu = (\mathbf{A}, Du)$ is exactly the Anzellotti's pairing between $\mathbf{A}$ and Du.

In the paper [3] we introduce a family of pairings between a bounded divergence-measure vector field and a function u of bounded variation, depending on the choice of the pointwise representative of u. The main ingredients to build this family of pairings are the absolute continuity of the measure $\mathrm{Div}\mathbf{A}$ with respect to the $(N-1)$-dimensional Hausdorff measure $\mathcal{H}^{N-1}$, and the fact that the pointwise value of a BV function can be specified up to a $\mathcal{H}^{N-1}$-negligible set. We prove that these pairings inherit from the standard one, all the main properties and features (e.g. coarea, Leibniz and Gauss–Green formulas). We also characterize the pairings making the corresponding functionals semicontinuous with respect to the strict convergence in BV.

All these extensions are motivated, among others, by applications to hyperbolic conservation laws and transport equations, problems involving the 1-Laplace operator, the prescribed mean curvature problem and to lower semicontinuity problems in BV.

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Fractional and anomalous diffusions on fractals

In recent years, there has been an increasing interest in studying stochastic processes and the corresponding operators on fractals. Initial interest in the properties of processes on fractals came from mathematical physicists working in the theory of disordered media: in fact certain media can be modelled by percolation clusters at criticality, which are expected to exhibit fractal-like prop- erties (see, for example, S. Havlin, D. Ben-Avraham, Diffusion in disordered media, Adv. Phys. 36, 695–798 (1987)).

Our studies focus on fractional and anomalous diffusions in fractals domains. More precisely, we study fractional equations, that is equations involving fractional operators in time and in space. We deal with time fractional equations in order to model anomalous diffusions, that is, diffusions with a non-linear relationship to time in which the mean squared displacement is propor- tional to a power $\beta \neq 1$ of time. For $\beta \in (0, 1)$ the anomalous diffusion exhibits a subdiffusive behavior (for example, due to particle sticking and trapping phenomena) whereas, for $\beta > 1$ we have superdiffusive behaviour (for instance, jumps). A type of space fractional equation we consider in our work is the one involving the fractional Laplacian, for instance. Equations involving time-space fractional derivative have been considered in order to model ground water flows and transport (fractional in space and example of superdiffusion), the motion of individual fluorescently labeled mRNA molecules inside live E. coli cells (fractional in time and example of subdiffusion). Further applications can be found in the theory of viscoelasticity, in modeling the cardiac tissue electrode interface, in modeling the anisotropies of the Cosmic Microwave Background radiation where the involved processes move on the sphere or, in general, on compact manifold.

We point out that many physical, biological, chemical and industrial processes are based on this dynamics on fractals. Indeed, many physical and biological phenomena take place across irregular and wild structures in which boundaries are "large", while bulk is "small" like for example organic molecules or metabolites in biological cells or brain tissue, particles in porous media, reactive species in porous catalysts, oxygen in human lungs, ions near rough electrodes or cellular membranes, water molecules in rocks, gas in fractures etc.

We studied fractional and anomalous diffusions on fractals by constructing suitable mathematical tools describing the fractional and/or anomalous diffusions and by providing a probabilistic treatment of the processes.

In the following figures we show examples of fractals domains (more precisely, random Koch domains) where we have focused our studies.

A key tool in the probabilistic approach is the time change of stochastic processes. In fact, we describe the anomalous diffusion by means of a suitable time change of diffusion process, for instance Brownian motion.

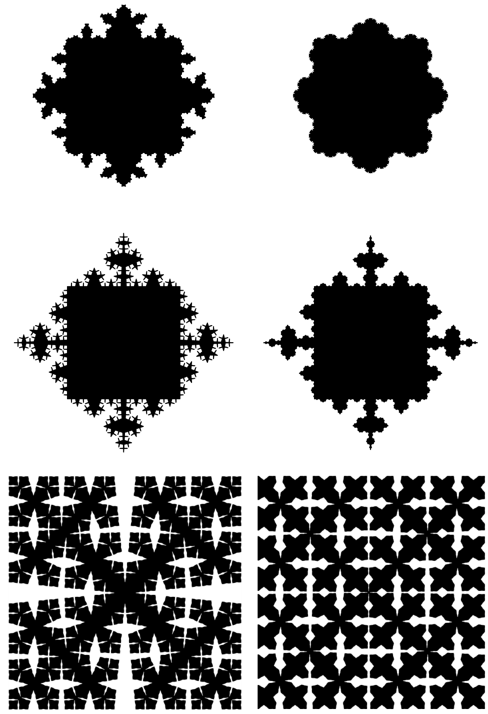

Figure 1: Random Koch domains

By using the theory of Dirichlet forms and the M-convergence we studied the connection between convergence of stochastic processes driven by time fractional equations and convergence of related forms. As the theory of Dirichlet forms provides an appropriate functional framework to the variational description of composite media and irregular structures like fractals, our results can be applied to several contexts and many areas. Thus, our results provide a useful tool for studying fractional equations in general scenarios.

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Problems involving 1-laplacian principal part

The main goal of this research is to deal with existence, regularity (and uniqueness, if attainable) of distributional solutions to problems involving the 1-laplacian as a principal part and a lower order terms which can become singular on the set where the solution u vanishes. Formally the problem looks like

$$\begin{cases} -\Delta_1 u := -\operatorname{div}\left(\dfrac{Du}{|Du|}\right) = h(u)f & \text{in } \Omega, \\ u \geq 0 & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where Ω is a bounded open subset of R^N with Lipschitz boundary, $0 \leq f \in L^N(\Omega)$, $h : [0, \infty) \to [0, \infty]$ is a continuous function, finite outside the origin, bounded at infinity and possibly unbounded near the origin $s = 0$ without any monotonicity property.

The natural space for this kind of problems is BV (or its local version BV_{loc}), the space of functions of bounded variation, i.e. the space of L^1 functions whose gradient is a Radon measure with finite (or locally finite) total variation. In (1) $\frac{Du}{|Du|}$ is the Radon-Nikodym derivative of the measure Du with respect to its total variation $|Du|$.

Problems involving the 1-laplace operator, which is known to be closely related to the mean curvature operator, enter in a variety of both practical and theoretical issues as for instance in image restoration and in torsion problems. We refer the interested reader to the monograph [1] for a more complete review on applications.

Let us first explain the meaning of solution in the particular non-degenerate case i.e. $0 < f \in L^N(\Omega)$. A function $u \in BV_{\text{loc}}(\Omega) \cap L^\infty(\Omega)$ will be a distributional solution to problem (1) if there exists an L^∞–divergence–measure vector field z, bounded by 1, such that in the distributional sense

$$-\operatorname{div} z = h(u)f.$$

This vector fied z satisfies $(z, Du) = |Du|$ as measures in Ω where (z, Du) is the so called Anzellotti pairing, playing in this way the role of the ratio $\frac{Du}{|Du|}$. Moreover the boundary condition has to be satisfied in a convenient weak sense by z and u.
In order to get existence, we require a smallness condition on the datum that f depending on the behavior of the function h at infinity, i.e.

$$||f||_{L^N(\Omega)} < \frac{1}{\mathcal{S}_1 h(\infty)}, \tag{2}$$

where $\mathcal{S}_1$ is the best constant in the Sobolev inequality for functions in $W_0^{1,1}(\Omega)$. Note that no smallness condition is assumed if $h(\infty) = 0$. This shows that the behavior of h at infinity can induce a first regularizing effect on the problem if compared to the non-singular case (e.g. $h \equiv 1$). A second regularizing effect appears if $h(0) = \infty$; the presence of a singular term will imply that $u > 0$ in Ω that is again in contrast with the non-singular case.
In this non-degenerate case further properties for solutions can be proved such as $h(u)f \in L^1(\Omega)$ and uniqueness in a suitable class of functions, if h is decreasing.

Let us consider now the case of a general nonnegative datum f, always assuming smallness condition (2).
If f can vanish on a subset of Ω of positive measure, the situation becomes much more delicate and it will involve the region $\{u > 0\}$ in an essential way. We will be forced to ask, in the definition of solutions to (1), that $\chi_{\{u>0\}} \in BV_{\text{loc}}(\Omega)$ where $\chi_{\{u>0\}}$ is the characteristic function of the region $\{u > 0\}$ and that the equation

$$-(\operatorname{div} z)\chi^*_{\{u>0\}} = h(u)f \tag{3}$$

is satisfied in the sense of distributions, where $\chi^*_{\{u>0\}}$ is its precise representative (in the sense of the BV–function).
One may observe that equation (3) can also be written as $-\operatorname{div}\left(z\chi_{\{u>0\}}\right) + |D\chi_{\{u>0\}}| = h(u)f$, where the term $|D\chi_{\{u>0\}}|$, is a measure concentrated on the reduced boundary $\partial^*\{u > 0\}$.
Moreover, as f is assumed to be merely nonnegative, we are only able to prove that $h(u)f \in L^1_{\text{loc}}(\Omega)$ (instead of $h(u)f \in L^1(\Omega)$ which holds true in the case of positive f) and no uniqueness of solutions holds.

The technique we exploit in order to get our existence results is the approximation with problems having p-laplacians principal part with $p > 1$.

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Singular and backward diffusion processes

This research line focuses on three carefully selected classes of nonlinear Partial Differential Equations (PDEs) with a highly nonlinear diffusion mechanism. All models have at the same time a novel structure and a robust connection to applications in Physics and Engineering. The general goal is to develop a thorough analysis, from well-posedness and regularity to qualitative properties and scaling laws.

Flux-saturating diffusion equations. This is a class of second-order parabolic equations of the form

$$\partial_t u = \operatorname{div} \mathbf{j}(u, \nabla u), \quad \lim_{t\to+\infty} \mathbf{j}(u, t\mathbf{v}) \cdot \mathbf{v} = u^m \quad \forall \mathbf{v} \neq 0 \quad (1)$$

with $m \geq 0$. The interest in this class is steadily growing, boosted by applications in physics and image processing. The flux saturation encoded by $(1)_2$ yields a (possibly nonlinear) *hyperbolic scaling* of $(1)_1$ in the regime of large gradients: hence $(1)_1$ is naturally set in BV-spaces and shares many features with nonlinear conservation laws. Among them, the most interesting one is probably the *formation of shocks* (i.e., jump discontinuities) in the bulk, which is expected and numerically observed for $m > 1$ (see Fig. 1). With the general goal of a rigorous

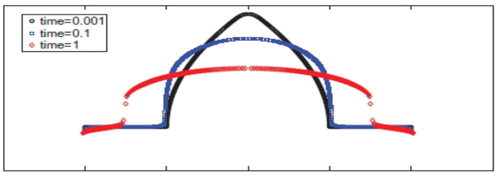


Figure 1: Numerical evidence of shock formation for (1) with $m = 4$ [Proc. London Math. Soc. 107 13951423 (2013)]

description of the saturation mechanism which triggers such formation, we are considering a prototype of (1) with purely hyperbolic scaling: $\mathbf{j}(u, \mathbf{v}) = u^m \mathbf{v}/|\mathbf{v}|$. We are currently working on its well-posedness and qualitative properties, based on our recent analysis of its resolvent equation [1].

1-harmonic flow. The 1-harmonic flow is the formal gradient flow (with respect to the L^2-distance) of the total variation TV of a function $\mathbf{u}$ from a domain Ω *to a Riemannian manifold* $\mathcal{N}$:

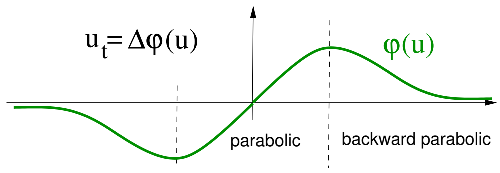
$$TV[\mathbf{u}] = \int_\Omega |D\mathbf{u}|, \qquad \partial_t \mathbf{u} = -\partial_{\mathbf{u}} TV[\mathbf{u}], \qquad \mathbf{u} \in \mathcal{N}.$$

The resulting PDE reads as

$$\partial_t \mathbf{u} - \operatorname{div}\left(\frac{D\mathbf{u}}{|D\mathbf{u}|}\right) = \mathcal{A}_{\mathbf{u}}\left(\partial_{x^i}\mathbf{u}, \frac{\partial_{x_i}\mathbf{u}}{|D\mathbf{u}|}\right), \quad \mathbf{u} \in \mathcal{N},$$

$\mathcal{A}$ being the second fundamental form of $\mathcal{N}$ (we use Einstein's summation convention). The 1-harmonic flow is an extremely powerful tool in denoising algorithms and has an intrinsic mathematical interest as prototype of constrained (on $\mathcal{N}$) gradient flows in BV-spaces. The final goal of our research, which started years ago with the case $\mathcal{N} \subseteq \mathbb{S}^{N-1}$, is to develop a theory for flows of BV-functions on a generic manifold $\mathcal{N}$. In order to gain insights, we recently studied simplified cases: unconstrained vector-valued flows in one-dimensional domains [2] and flows on $\mathcal{N}$ of Lipschitz functions [3].

Forward-backward parabolic equations. The description of temperature stratification in the ocean, aggregation phenomena in biology, and Perona-Malik diffusion in image processing, all lead to evolution equations which are forward, resp. backward, parabolic for small, resp. large values of the unknown: In view of the back-



ward parabolic character, these equations are ill-posed and singularities (e.g., Dirac measures) are doomed to form. Various types of regularisation have therefore been proposed, on which the qualitative properties of solutions is expected to depend. In [4] we designed a new, *nonlinear fourth-order regularization*, which we show to admit *solutions with singularities that can both appear and disappear*. We believe that these features will permit a better description, e.g. in term of time-scales, of key phenomena which are commonly observed in numerical approximations to the equation, such as the early-stage formation of wrinkling-type singularities followed by a coarsening process.

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Characterization results for the solutions of the Lane-Emden equation

Lane-Emden type equations are extremely simple looking semilinear elliptic equations with a power focusing nonlinearity. They are a model case for the study of more general families of equations, furthermore they are used in astrophysics to model self-gravitating spheres of plasma, such as stars or self-consistent stellar systems.
Despite their simple appearance, they have a very rich mathematical structure in terms of the dependance of the solutions on the exponent p of the power nonlinearity and on both the geometry and the topology of the domain.
The research activity focused on the study of existence, multiplicity/uniqueness and qualitative properties of the solutions to these equations, in dependance of both the power p and the domain.
We have considered the 2-dimensional case, for which very few results were available in the literature, addressing the following main topics:

- *Uniqueness of the positive solution for the Dirichlet boundary problem in any convex bounded domain*
  This was a longstanding open problem which arose in the seminal paper [Gidas, Ni, Nirenberg, CMP 1979] and was conjectured to be true already in [Kawhol, Lect. Notes in Math. 1985] and [Dancer, JDE 1988]. Only partial results where know: some considering specific domains (balls, perturbations of the ball, domains with some additional symmetry, etc) and other considering specific families of solutions (for instance least energy ones).
  We have completely solved the conjecture when p is sufficiently large (see Ref. 2.).

- *Asymptotic characterization as $p \to +\infty$*
  It is known that in dimension $N \geq 3$ solutions may blow-up when p approaches the critical Sobolev exponent and this behavior is nowadays well characterized (see e.g. [Struwe, Math.Z. 1984], [Schoen, Lect. Notes 1988-1989], [Han, Ann.Inst.H.Poincare, 1991]). On the contrary in dimension 2 the behavior of the solutions as $p \to +\infty$ was essentially an open problem and only specific cases of solutions had been previously described (e.g. least energy solutions).
  We have obtained a complete characterization of the asymptotic behavior of the positive solutions as p goes to $+\infty$ for the Dirichlet boundary problem in any smooth bounded planar domain (see e.g. Ref. 1. and Ref. 3.).
  In simple words we have shown that any family of bounded energy solutions concentrate at a finite number of distinct points, moreover differently than in the higher dimensional case they do not blow-up but remain bounded (*multi-peak solution*). We have also characterized the concentration set, the *limit profile* around each point and proved that an energy quantization holds. For sign-changing solutions, we can prove that they also must concentrate at a finite number of points, but different phenomena may appear and a complete general characterization seems to be a very hard task to be carried out in this case. Nevertheless we have characterized the concentration behavior of all the radial solutions in the unit ball, for which a *tower* of different limit profiles appears at the same point. This result could be useful also to get multiplicity results in more general domains.

- *Morse index computation and non-degeneracy*
  Computing the Morse index of a solution or having at least an uniform bound of it is, in general, not an easy issue, but its knowledge can be useful both for deducing uniqueness and multiplicity results. For Lane-Emden equations the Morse index and the non-degeneracy were known for least-energy solutions and, under symmetry assumptions, some Morse index estimates were available.
  We have investigated these topics, in particular we have computed the Morse index when p is large, both for positive and radial solutions, by strongly exploiting the asymptotic analysis described at the previous point (see e.g. Ref. 2.).

- *Multiplicity results*
  For the Dirichlet problem in the ball numerical results in the literature surprisingly suggested the existence of sign-changing nonradial solutions bifurcating from the branches of the radial solutions at certain values of the exponent p.
  We have found these solutions combining the information given by the exact computation of the Morse index (previous point), with suitable spectral decompositions and blow-up analysis (see Ref. 4.).

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Mathematical modeling and control of an octopus arm

Contribution to the Scientific Report 2018-2020 of the Department of Basic and Applied Sciences for Engineering, Sapienza University of Rome.

Octopus arms are complex, fascinating biological structures that attracted the interest of researchers in both natural science as well as in bio-inspired robotics, in particular, in the framework of soft manipulators [1]. In [2] a mathematical control model for octopus arm is introduced in order to describe the voluntary muscle contractions of the tentacle and to derive optimality conditions for a reachability problem. More precisely, the tentacle is modeled as a three-dimensional body with an axial symmetry, with a fixed endpoint, and characterized by longitudinal inextensibility: the aim is to investigate the evolution of the curve on the plane representing the symmetry axis. The symmetry axis is assumed to be a string subject to the following constraints:

- inextensibility: the octopus arm can bend but not stretch longitudinally;
- bending moment: the soft structure resists to bending via an angular elastic potential with non-uniform elastic constant ε;
- curvature constraint: the arm cannot bend over a fixed threshold ω;
- curvature control: a time-varying, internal angular elastic force, with non-uniform elastic constant μ, is applied in order to pointwise force the bending of the arm.

The inextesibility constraint is imposed exactly, whereas the bending moment, the curvature constraint, and the curvature control are introduced by a penalty method. Starting from a discrete particle system, we encode all of the geometrical constraints into a discrete Lagrangian for the system, then we obtain the continuous model as a formal limit for the number of particles going to infinity. The resulting continuous Lagrangian, depending on the arm axis configuration q and of the tension σ (which is the Lagrange multiplier associated to the exact inextensibility contraint), is the following

$$\begin{aligned}\mathcal{L}(q,\sigma) := \int_0^1 \Big(& \underbrace{\frac{1}{2}\rho|q_t|^2}_{\text{kinetic en.}} - \underbrace{\frac{1}{2}\sigma(|q_s|^2-1)}_{\text{inextensibility constr.}} \\ & - \underbrace{\frac{1}{4}\nu\left(|q_{ss}|^2-\omega^2\right)_+^2}_{\text{curvature constr.}} \\ & - \underbrace{\frac{1}{2}\varepsilon|q_{ss}|^2}_{\text{bending mom.}} - \underbrace{\frac{1}{2}\mu\left(\omega u - q_s \times q_{ss}\right)^2}_{\text{curvature control}} \Big) ds\,,\end{aligned}$$

The equations of motion are obtained by the least action principle and result in an evolutive, fourth-order, non-linear system of control partial differential equations generalizing the *dynamic Euler's elastica equation*. The equilibrium configurations are characterized. Then, the following optimal control problem is addressed: to steer the tentacle tip to a target point while minimizing the activation of the tentacle muscles. More precisely, we want to optimize the distance of the tentacle tip from a fixed target point and a quadratic cost associated to the controls. This is done in two different settings, a stationary case and a dynamic case. In the stationary case, it is established a relation with a classical problem first posed by Markov in 1887, also known as the *Dubins car problem*. In the dynamic case, the objective functional accounts for the whole evolution of the tentacle on a time interval $[0, T]$, plus a term representing the kinetic energy at the final time T. The aim then is also to stop the tentacle as soon as possible. To this end, we introduce an adjoint state and derive first order optimality conditions. The resulting optimality system is then solved numerically via an adjoint-based gradient descent method.

In [3], the above described model is declined in the context of soft robotics and it is also considered the possibility that a subregion of the arm is not controlled, motivated by possible mechanical breakdowns or energy saving purposes. Stationary and dynamic optimal reachability problems are addressed and numerically solved. In [4] we performed a deeper investigation of the model and of its connection with hyper-redundant manipulators. The important problem of grasping a prescribed object is addressed in a stationary setting. Our approach, involving the theory of optimal control of PDEs, allows in a quite natural way for an extension to fully dynamic optimization.

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Scalar and vector BVPs on extension domains: theory and applications

Many engineering models are characterized by the presence of different temporal and spatial scales and/or by the presence of contacts among different components through rough (fractal) interfaces. These barriers or boundaries are often highly irregular. In quite all these phenomena the information flows from a smaller to a larger scale or viceversa. Fractals provide a useful tool to describe such wild geometries. A great challenge is to propose mathematical models which allow investigating these phenomena with a particular regard to scale effects and interface interactions as well as their numerical approximation.
The first examples in the literature in which classical BVPs merge with the theory of fractal sets and operators are due our group in 2002. Numerical approximation of BVPs in domains with fractal boundaries or interfaces, which model fast heat diffusion phenomena across a Koch interface, is more recent. Nevertheless, many problems are still open, but at the same time, from the point of view of applications, rigorous formulations and models for vector BVPs are strongly demanding. We investigated some scalar and vector BVPs for heat flow, magnetostatics and fluid dynamics, possibly with non-standard boundary conditions. We stress the fact that, when dealing with vector fields in fractal domains, it is necessary to introduce new tools and techniques.

In [1] we studied the following Venttsel' problem:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \mathcal{L}[u] = f & \text{in } \Omega, \\ \dfrac{\partial u}{\partial t} + \dfrac{\partial u}{\partial \nu_{\mathcal{L}}} - \mathcal{L}_{\partial\Omega}[u] + bu + \Theta(u) = g & \text{on } \partial\Omega, \\ u(0,x) = u_0(x) & \text{in } \overline{\Omega}, \end{cases}$$

where $\mathcal{L}$ is a general linear differential operator, Θ is a nonlocal operator and Ω is a 2D domain with fractal (or pre-fractal) boundary. The peculiarity of Venttsel' problems is that the operator $\mathcal{L}$ acting in the bulk has the same order of the operator $\mathcal{L}_{\partial\Omega}$ acting on the boundary. We proved existence and uniqueness for the weak solution via a semigroup approach as well as regularity results in weighted Sobolev spaces. These results are crucial to obtain optimal error estimates when considering the numerical approximation by FEM in space and finite difference in time (see Fig. 1). The results show that the presence of a fractal interface enhances the absorption effects of the layer, which acts as a preferential fast absorbing trail for the heat stream.

In [2] we proved Gaffney inequality for extension domains. Gaffney inequality is a crucial tool in proving coercivity estimates for the associated energy functionals e.g. for Navier-Stokes and Maxwell equations. In [3] we studied a magnetostatic problem in a 3D fractal domain. We gave a suitable notion of tangential trace for a vector field via a generalized Stokes theorem and then, by Gaffney inequality, we proved existence and uniqueness of weak solutions as well as regularity results. We studied also the corresponding pre-fractal problems and we proved that the pre-fractal solutions converge to the limit fractal one. These results are crucial in view of the numerical approximation by FEM (see Fig. 2).

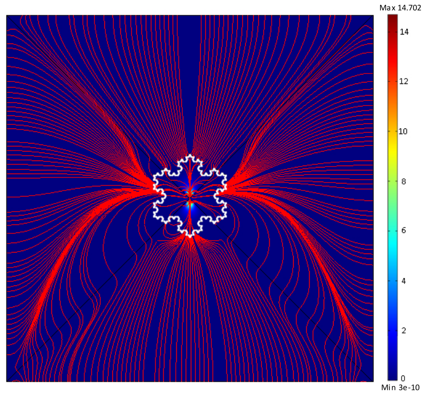

Figure 1: Stationary streamlines.

In [4] we proved existence and uniqueness results, by a semigroup approach, for the unsteady Stokes problem with no-slip boundary conditions in fractal and pre-fractal cylinders. We studied the asymptotic behavior of the pre-fractal solutions via the M-convergence of the energies. The convergence of the approximating pressures was also investigated.

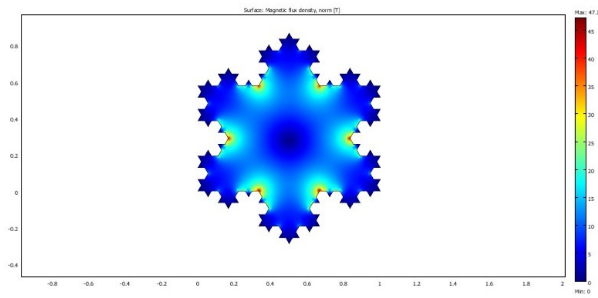

Figure 2: Magnetic field generated inside a pre-fractal domain.

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M. R. Lancia, S. Creo.

Comparison principle for unbounded solutions of elliptic and parabolic equations with first order terms

Let $\Omega \subset \mathbb{R}^N$, $N > 2$, be a bounded domain and let $A(x) = (a_{i,j}(x))$ be a coercive matrix of bounded functions. We are interested in studying the uniqueness of unbounded solutions to the elliptic problem

$$\begin{cases} u - \operatorname{div}(A(x)Du) = H(x, Du) & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega \end{cases} \tag{1}$$

where $H(x, Du)$ is measurable with respect to x, locally Lipschitz with respect to ξ and has a super linear growth with respect to the gradient, namely

$$|H(x,\xi)| \le \gamma|\xi|^q + f(x) \tag{2}$$

for a.e. $x \in \Omega$ and every $\xi \in \mathbb{R}^N$, for some $q > 1$ and $f(x)$ belonging to some Lebesgue space $L^m(\Omega)$.

It is well known that, if $\xi \mapsto H(x,\xi)$ is locally Lipschitz and has at most linear growth, then problem (1) admits a unique weak solution in the Sobolev space H_0^1. This is no longer true in case of super linear growth of the first order terms, and uniqueness may fail. For example, the function

$$u(x) = c_{q,N}\left(|x|^{-\frac{2-q}{q-1}} - 1\right)$$

is a nontrivial solution of the problem

$$\begin{cases} -\Delta u = |Du|^q & \text{in } B_1(0), \\ u = 0 & \text{on } \partial B_1(0), \end{cases}$$

in the distributional sense, if $N/(N-1) < q < 2$ and for a suitable choice of the constant $c_{q,N} > 0$. In particular, this is also a non trivial $H_0^1(\Omega)$ solution if $1 + \frac{2}{N} < q < 2$.

This shows that the comparison principle does not hold straightforwardly for elliptic equations with super linear first order terms in the class of unbounded solutions, so this issue should be handled with care.

We found sufficient conditions in order to have a comparison principle among unbounded sub and super solutions to (1) in a suitable class of functions.

Indeed, if we suppose that $H(x,\xi)$ is a Carathéodory function such that $\xi \mapsto H(x,\xi)$ is locally semi-convex, namely

$$\forall\ K > 0 \quad \exists\ c_K\ :\ \xi \mapsto H(x,\xi) + c_K|\xi|^2$$

is convex in $B_K(0) := \{\xi \in \mathbb{R}^N : |\xi| \le K\}$ and, in addition, $H(x,\xi)$ is convex at infinity, namely

$$\exists\, R > 0 : \quad \xi \mapsto H(x,\xi)$$

is convex in $B_R(0)^c := \{\xi \in \mathbb{R}^N : |\xi| > R\}$, then a comparison principle holds true, if (2) is in force with $1 + \frac{2}{N} \le q < 2$ and $f \in L^{\frac{N}{q'}}(\Omega)$, in the class of functions such that

$$(1 + |u|)^{\sigma - 1} u \in H^1(\Omega)$$

with $\sigma = \frac{(N-2)(q-1)}{2(2-q)}$.

In particular, under the above assumptions, problem (1) has a unique solution in such a class.

The same type of phenomenon has been studied for unbounded sub/supersolutions to parabolic equations of the type

$$\begin{cases} u_t - \Delta_p u = H(t,x,Du) + f(t,x) & \text{in } \ (0,T) \times \Omega, \\ u(t,x) = 0 & \text{on } \ (0,T) \times \partial\Omega, \\ u(0,x) = u_0(x) & \text{in } \ \Omega, \end{cases}$$

where $T > 0$ and u_0 belongs to a suitable Lebesgue space. Here $-\Delta_p u$ denotes the p–Laplacian, and H satisfies suitable growth assumptions on the last variable.

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FOURIER SERIES AND CONTROL THEORY

Contribution to the Scientific Report 2018-2020 of the Department of Basic and Applied Sciences for Engineering, Sapienza University of Rome

- **Alternating and variable controls for the wave equation.** The problem of observability for the wave equation with Dirichlet boundary conditions is one of the first topic in the theory of observability and controllability for distributed systems: usually in the one dimensional case the observability set is $\{0\} \times (0, T)$ or $\{\pi\} \times (0, T)$. In the work [1] the idea is to generalize the situation of having different observability set and to alternate the spatial point still maintaining the observability inequality true, in an optimal control time. More precisely, $\Omega = (0, \pi)$ and we consider the system

$$u_{tt} - \Delta u = 0\,, \qquad (x,t) \in \Omega \times (0,T)\,, \quad (1)$$
$$u(x,t) = 0\,, \qquad (x,t) \in \partial\Omega \times (0,T)\,, \quad (2)$$
$$u(x,0) = u_0(x)\,, \qquad x \in \Omega\,, \quad (3)$$
$$u_t(x,0) = u_1(x)\,, \qquad x \in \Omega\,; \quad (4)$$

and we say that (**??**)-(**??**) is $\mathcal{F}$-observable, if the system is $\mathcal{F}$-observable for some time $T > 0$.
Suppose that the system (**??**)-(**??**) is $\mathcal{F}$-observable in time T, but it is not $\mathcal{F}$-observable in any time $T' < T$. Then $T_{opt} := T$ is called the *optimal control time*. Observability inequalities are obtained by the Fourier method. Some results are also obtained in the multidimensional case.

- **Simultaneous observability and controllability of systems of strings and beams.** There have been many results during the last twenty years on the simultaneous observability and controllability of systems of strings and beams, see [3] for detailed references. Observability of vibrating strings, membranes, beams and plates has also been investigated intensively by several different methods (multipliers, Fourier, and microlocal analysis).
Controllability and observability are dual aspects of the same problem: deep mathematical tools arise trying to solve the problems of observability and controllability. Many of them have an independent interest, and they can be formulated in an abstract setting.
The approach in [2] also allows to consider infinite systems of beams, which requires a deeper study of the overall density of the union of all corresponding eigenfrequencies. For infinite systems of beams we also show that, in some particular cases, we may do an accurate computation under some algebraic conditions on the lengths of the beams. As example, recalling that a Perron number is a real algebraic integer q of degree ≥ 2 whose conjugates are all smaller than q in absolute value (the Golden Ratio $q \approx 1.618$ is a Perron number), the detailed analysis is given when beam-length$(j) = q^{-j}$, with q Perron number.

- **Glass relaxation models: a viscoelastic approach.** Motivated by applications, and increasing interest devoted to glass materials concerned with high-tech applications regarding the best possible performances for computer displays, we studied the equation of viscoelasticity to model the behavior of glass relaxation.
Viscoelasticity is the property of materials that exhibit both viscous and elastic characteristics and for some glass relaxation models the stretched exponential function, obtained by inserting a fractional power into the exponential, has been proposed as stress relaxation modulus.
Taking advantage of the approximation of the stretched exponential function with a general Prony series in glass relaxation, in the paper [4] the spectral analysis for the equation of viscoelasticity is studied.
In order to obtain more precise results, simplification of the equation is necessary. Mechanical models involving springs and dashpots are used to explain the creep and the Burgers model is a typical model which combine a series of elements with springs and dashpots and describe the case in which a Maxwell and a Kelvin-Voigt model are connected in series. Burgers model is a simplification, indeed the corresponding equation of the viscoelasticity has as memory kernel a Prony series with two terms. For the Burgers model we are able to perform a complete and detailed spectral analysis. A study of the asymptotic behavior of all eigenvalues allows us to represent the solution of the integro-differential equation as a Fourier series.

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P. Loreti, D. Andreucci, A. C. Lai, D. Sforza.

Elliptic and parabolic singular boundary value problems

Let Ω be a bounded and smooth open subset of $\mathbb{R}^N$, and consider, as a model, the following singular elliptic boundary-value problem

$$\begin{cases} -\Delta u = \dfrac{f}{u^\gamma} & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \qquad (1)$$

where $\gamma > 0$, and f is a nonnegative function.

Physical motivations in the study of problems as (**??**) arise, for instance, in the study of thermo-conductivity where u^γ represents the resistivity of the material, in signal transmissions, and in the theory non-Newtonian pseudoplastic fluids (see [1] and references).

From the purely theoretical point of view, after some first pioneering existence and uniqueness results, a systematic treatment of problems (**??**), also called singular Lane–Emden–Fowler, was developed in the seventies.

If f is smooth enough (say Hölder continuous) and bounded away from zero on Ω then the existence and uniqueness of a classical solution to (**??**) is proven by desingularizing the problem and then by applying a suitable sub- and super-solution method. Some remarkable refinements of the previous results were given in [2]; here, the authors proved, in particular, that $u \notin C^1(\overline{\Omega})$ if $\gamma > 1$ and it has finite energy, i.e. $u \in H_0^1(\Omega)$, if and only if $\gamma < 3$.

Consider now a more general the boundary-value problem of the form

$$\begin{cases} -\Delta u = h(u)f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \qquad (2)$$

where $h : \mathbb{R}^+ \to \mathbb{R}^+$ is a continuous function that may blow up at $s = 0$ and possesses a limit at infinity, and f is a nonnegative function in $L^1(\Omega)$ (or, possibly, a bounded Radon measure on Ω).

Besides the one arising from the presence of possibly a measure datum, new difficulties have to be taken into account in this general framework; even if f is only a nonnegative function, then the solutions do not belong in general to $H_0^1(\Omega)$ even for small γ.

In addition, the lower order term in (**??**) need to belong to $L^1(\Omega)$ in general; the question of the summability properties of the lower order term in (**??**) plays a crucial role in order to deal with uniqueness of solutions. In general, in fact, only finite energy solutions are known to be unique, at least in the model case (**??**).

In [3], under fairly general assumptions we introduced a natural notion of distributional solution to problem (**??**) for which existence can be shown to hold. Moreover, uniqueness holds provided h is nonincreasing. Particular care is addressed on how the homogeneous boundary datum for the solution u is (weakly) attained.

If f is a function in $L^m(\Omega)$, $m \geq 1$, we also investigate the question of whether the solution to problem (**??**) has finite energy. We provide several instances of this occurrence depending on the regularity of the datum and on the behavior of $h(s)$ both at zero and at infinity. A typical (sharp) statement said that a finite energy solution does exist for ani $f \in L^m(\Omega)$ if and only if

$$\gamma < 3 - \frac{2}{m}\,,$$

which fits with the result in [2] as $m \to \infty$ (that is as f becomes smoother).

Additionally, we obtain sharp thresholds for the lower order term to belong to $L^1(\Omega)$. The results and their optimality are discussed through appropriate examples.

Also, we finally establish a weighted summability estimate on the lower order term $h(u)f$; this will be a key tool in order to prove uniqueness, which will be obtained by mean of a suitable Kato type inequality.

The parabolic counterpart of problems as in (**??**) has been faced in [4]; here we consider nonnegative integrable data f and u_0, a nonnegative bounded Radon measure as nonhmogeneous source and a merely continuous, and possibly singular at the origin, nonlinear zero-order term $h(s)$. Under these general assumptions we prove existence of a nonnegative solution for problem

$$\begin{cases} u_t - \Delta u = h(u)f + \mu & \text{in } \Omega \times (0,T), \\ u = 0 & \text{on } \partial\Omega \times (0,T), \\ u = u_0 & \text{in } \Omega \times \{0\}, \end{cases}$$

and uniqueness of finite energy solutions (in the homogeneous case) provided h is nonincreasing. Same type of result are extended to the case of equations with a quasilinear p-laplace type leading term as

$$u_t - \Delta_p u = h(u)f + \mu \quad \text{in } \Omega \times (0,T)\,.$$

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Authors

F. Petitta, F. Oliva

Numerical Solution of Fractional Differential Equations

In recent years fractional calculus has been used in several fields to model real-world phenomena. Integro-differential equations of *fractional*, *i.e.* positive real, order are used, for instance, to model wave propagation in porous materials, diffusive phenomena in biological tissue, viscoelastic properties of continuous media [1]. Even if these models are empirical, nevertheless they are shown to be consistent with experimental data.
The increased interest in fractional models has led to the development of several numerical methods to solve fractional integro-differential equations. In [2] we proposed a collocation method especially designed for solving differential equations of fractional order. The key ingredient of the method is the use of the fractional splines [3] as approximating functions. Thus, the method takes advantage of the explicit differentiation rule for fractional B-splines that allows us to evaluate accurately the derivatives of both integer and fractional order. The method was used to solve multi-term differential equations [2], time-fractional differential diffusion problems [4,5], nonlinear fractional differential problems [6,7], boundary value problems having space derivative of fractional order [8].

Here, we show the numerical results we obtained in [9]. Consider the *time-fractional dynamical system*

$$\begin{cases} D_t^\gamma X(t) = A\, X(t)\,, \qquad t > 0\,, \quad 0 < \gamma < 1\,, \\ \\ X(0) = X_0\,, \end{cases} \tag{1}$$

where $X(t) : \mathbb{R} \to \mathbb{R}^m$ is a real-valued vector function, $X_0 \in \mathbb{R}^m$ is a real vector and $A \in \mathbb{R}^{m\times m}$ is a real matrix. The operator D_t^γ denotes the *Caputo fractional derivative* with respect to the time t. For a sufficiently smooth vector function $X(t) = [x_1(t), x_2(t), \ldots, x_m(t)]^T$, its Caputo derivative is given by

$$D_t^\gamma X(t) := \left[D_t^\gamma x_1(t), D_t^\gamma x_2(t), \ldots, D_t^\gamma x_m(t)\right]^T\,, \tag{2}$$

where $D_t^\gamma x(t)$, $0 < \gamma < 1$, is defined as

$$D_t^\gamma\, x(t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{x'(\tau)}{(t-\tau)^\gamma}\, d\tau\,, \qquad t \geq 0\,, \tag{3}$$

Here, Γ denotes the Euler's gamma function.

We approximated the solution to differential problems (1) using the *fractional collocation method* introduced in [2]. The method was proved to be convergent with approximation order γ. Moreover, the numerical tests show that the method is efficient and accurate.

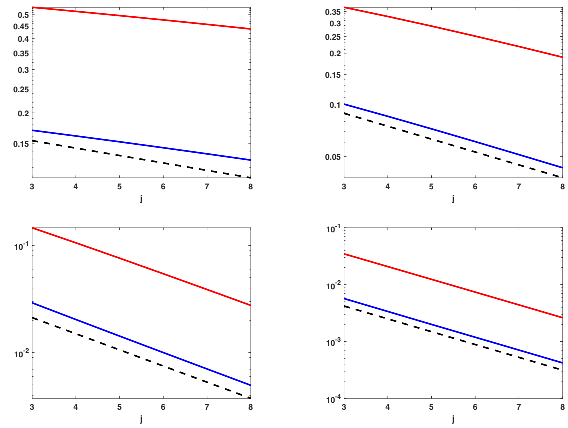

Figure 1: The numerical error as a function of the time step $h = 2^{-(j+1)}$ for $\gamma = 0.10$ (left top panel), 0.25 (right top panel), 0.50 (left bottom panel), 0.75 (right bottom panel) using the cubic spline (red line) and the spline of degree 4 (blue line). The black dashed line has the same slope as the theoretical error.

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L. Pezza, F. Pitolli

Phase separating solutions for two component systems

The Gross–Pitaevskii system [5, 8] consisting of two coupled nonlinear Schrödinger equations,

$$\begin{cases} \iota \dfrac{\partial}{\partial t}\Phi_j + \Delta\Phi_j - V_j(x)\Phi_j - \mu_j|\Phi_j|^2\Phi_j - \sum_{i\neq j}\beta_{ij}|\Phi_i|^2\Phi_j = 0 \\ \Phi_j = \Phi_j(x,t) \in \mathbb{C}, \\ \Phi_j(x,t) = 0,\ x \in \partial\Omega,\ j = 1,2 \end{cases} \tag{1}$$

is a mathematical model for the binary Bose–Einstein condensate for the unknown condensate wave functions Φ_j, $j = 1, 2$. Here Ω is a bounded smooth domain in $\mathbb{R}^2$, and the nonnegative constants μ_j's and $\beta'_{ij}s$ are the intraspecies and interspecies scattering lengths which represent the interactions between like and unlike particles, respectively. Hereafter, it is natural to assume that β_{ij}'s are symmetric, i.e. $\beta_{ij} = \beta_{ji}$ if $j \neq i$. The functions $V_j(x)$, $j = 1, 2$, represent the magnetic trapping potentials. To find solitary wave solutions of the system (1), we set $\Phi_j(x,t) = e^{-\iota\lambda_j t}u_j(x)$, $\lambda_j \in \mathbb{R}$ and $u_j \in \mathbb{R}$. Then we may transform the system (1) into a system of semilinear elliptic equations given by

$$\begin{cases} -\Delta u_j + (V_j(x)+\lambda_j)u_j = \mu_j u_j^3 + \sum_{i\neq j}\beta_{ij}u_i^2 u_j,\ x \in \Omega, \\ u_j(x,t) = 0,\ x \in \partial\Omega \quad j = 1,2, \end{cases} \tag{2}$$

which are time independent vector Gross-Pitaevskii/Hartree-Fock equations [3, 4] for the condensate wave functions u_j. It was shown in [13] that there are two distinct scenarios of spatial separation: (i) potential separation, caused by the external trapping potentials in much the same way that gravity can separate fluids of different specific weight; (ii) phase separation, which persists in the absence of external potentials. In the fluid analogy, phase separated condensates can be compared to a system of two immiscible fluids, such as oil and water.

Actually, in a binary mixture of Bose–Einstein condensates in the absence of external potentials, i.e. $V_i = 0$, a segregation phenomena occurs when intra species scattering lengths μ_j are constants and the parameter $\beta := \beta_{12}$ is large. In this case the two states repel each other and form segregated domains like the mixture of oil and water. Such a phenomenon is called phase separation of a binary mixture of Bose–Einstein condensates and has been investigated extensively by experimental and theoretical physicists ([5, 6, 13]). From a mathematical point of view, a lot of work has been done to study the segregation phenomena ([1, 2, 9, 10, 11, 12]). In particular, in [7] the authors find the governing equations of the limiting functions of the bound state solutions of the system (2) as $\beta \to \infty$: if $u_{1,\beta}$ and $u_{2,\beta}$ are $L^\infty(\Omega)-$uniformly bounded solutions of

$$\begin{cases} -\Delta u_{1,\beta} + \lambda_1 u_{1,\beta} = \mu_1 u_{1,\beta}^3 - \beta u_{1,\beta}u_{2,\beta}^2 & \text{in } \Omega, \\ -\Delta u_{2,\beta} + \lambda_2 u_{2,\beta} = \mu_2 u_{2,\beta}^3 - \beta u_{2,\beta}u_{1,\beta}^2 & \text{in } \Omega, \\ u_{1,\beta} = u_{2,\beta} = 0 \text{ on } \partial\Omega. \end{cases} \tag{3}$$

then, up to a subsequence, as β approaches $+\infty$ they converge in $C^{0,\alpha}(\overline{\Omega}) \cap H^1(\Omega)$ to a pair of functions u_1 and u_2 having compact disjoint supports (namely $u_1 u_2 \equiv 0$ in Ω) which solve

$$\begin{cases} -\Delta u_1 + \lambda_1 u_1 = \mu_1 u_1^3 & \text{in } \Omega \cap \{u_1 > 0\}, \\ -\Delta u_2 + \lambda_2 u_2 = \mu_2 u_2^3 & \text{in } \Omega \cap \{u_2 > 0\}, \\ u_1 = 0 \text{ on } \partial(\Omega \cap \{u_1 > 0\}),\ u_2 = 0 \text{ on } \partial(\Omega \cap \{u_2 > 0\}). \end{cases} \tag{4}$$

It is quite natural to ask if any solutions to the limiting equation (4) can be seen as the limiting functions of a bound state solutions of the system (3). In collaboration with Michał Kowalczyk (Universidad de Chile) and Giusi Vaira (Università di Bari) we address this question and give a positive answer in the paper *Phase separating solutions for two component systems in general planar domains* (submitted).

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Authors

A. Pistoia

Random methods for the solution of the M/EEG inverse problem

Neuroimaging aims at reconstructing the neuronal activity generated in the working brain using imaging techniques like functional Magnetic Resonance (fMRI), Positron Emission Tomography (PET), Electroencephalography (EEG), Magnetoencephalography (MEG). In particular, EEG and MEG are non-invasive techniques that measure the electric potential difference on the scalp and the magnetic field outside the head due to neuronal activations, respectively. The brain areas activated during sensory stimulation, cognitive processing or simply at rest can be inferred by electric and/or magnetic measurements. The solution to this ill-posed, ill-conditioned inverse problem requires regularization techniques that are often time-consuming and computationally and memory storage demanding [1], especially if we consider the new trends in EEG and MEG communities where the real time analysis and the employment of portable devices are gaining an increasing interest [2-4]. In [5] a procedure based on random sampling was introduced to significantly reduce the dimension of the EEG/MEG inverse problem thus reducing both memory usage and computation time. The key idea is to randomly select a few hundreds of points in the source space, which is the discretization space where the neuroelectric current is approximated. In [6] the random sampling was tested on both synthetic data and real MEG measurements to investigate how the source space reduction affects the localization accuracy of well-established inverse algorithms.

The numerical tests in [6] show that the random sampling method highly reduces the computational cost while the random selection procedure does not compromise the capability of detecting neural sources. The accuracy is higher in case of superficial sources while for deep sources the accuracy can be improved using regularization techniques specially suited for this case.

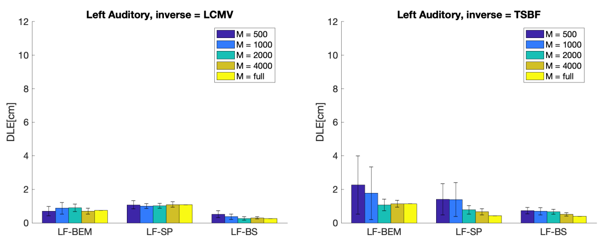

Figure 1: Left auditory evoked field: Mean Distance Localization error (DLE [cm]) and standard deviation obtained averaging over 10 runs of the random sampling method using two beamforming techniques (left panel: LCMV; right panel: TSBF). The forward problem was solved by the Boundary Element Method (BEM), the spherical model (SP) and the discretization of the Biot-Savart operator (BS).

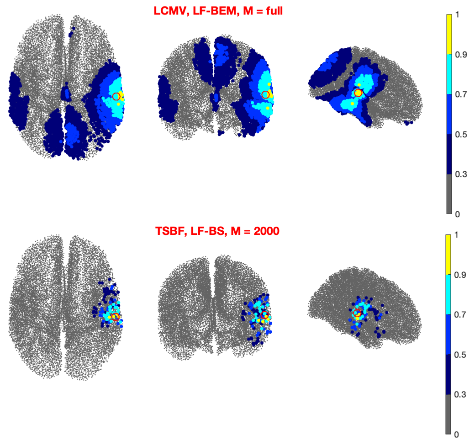

Figure 2: Left Auditory evoked field: The intensity of the estimated sources, averaged over 10 runs, at 90 ms obtained using LMCV and the BEM on the full source space (top panel) and TSBF and the BS on 2000 samples of the source space (bottom panel). The red circle shows the manually reconstructed source.

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Authors

F. Pitolli

Geometric bounds for the eigenvalues of the p-Laplacian

A classical result in spectral geometry is the following upper bound for the eigenvalues $\{\lambda_k\}_{k\in\mathbb{N}}$ of the Neumann Laplacian on a domain Ω of $\mathbb{R}^n$:

$$\lambda_k \leq C_n \left(\frac{k}{|\Omega|}\right)^{\frac{2}{n}}. \tag{1}$$

Here $|\Omega|$ is the Lebesgue measure of Ω, and C_n is an explicit constant depending only on n. The behavior in k agrees with the Weyl's law for λ_k. The result is due to Kröger and follows from an asymptotically sharp bound on eigenvalue averages. Its proof makes use of harmonic analysis on $\mathbb{R}^n$.

If we consider the *variational* eigenvalues of the Neumann p-Laplacian $\{\lambda_{k,p}\}_{k\in\mathbb{N}}$, we immediately realize that the classical theory for upper bounds does not apply, essentially because the lack of a Hilbert space structure prevents the use of harmonic analysis techniques.

In this setting, we recognize that a geometric approach is more suitable to treat the problem. In fact, already for the Laplacian case (i.e., $p = 2$), Kröger-type upper bounds on domains of a generic Riemannian manifold were unknown until B. Colbois, D. Maerten, J. Geom. Anal. 18 (2008), where the authors introduce a geometric technique based on the decomposition of a metric measure space by capacitors, in the spirit of N. Korevaar, J. Diff. Geom. 37 (1993) and P. Buser, Math. Z. 165 (1979).

The generality and versatility of the approach make it suitable to study the eigenvalues $\{\lambda_{k,p}\}_{k\in\mathbb{N}}$ on domains of complete n-dimensional Riemannian manifolds, and on compact manifolds, and look for bounds of the form (1). This is what we have done in [1].

As expected, one has to take into account the interplay of p and the space dimension n. The results can be declined in several directions. Let Ω be a bounded domain in a Riemannian manifold M with a metric g belonging to the conformal class $[g_0]$ of a fixed metric g_0 with $\mathrm{Ric}_{g_0} \geq -(n-1)\kappa^2$, and let $\{\lambda^g_{k,p}\}_{k\in\mathbb{N}}$ be the eigenvalues of the Neumann p-Laplacian on Ω with respect to the metric g. We prove in [1] that, if $1 < p \leq n$, then

$$\lambda^g_{k,p} \leq A_{p,n}\kappa^p \left(\frac{|\Omega|_{g_0}}{|\Omega|_g}\right)^{\frac{p}{n}} + B_{p,n}\left(\frac{k}{|\Omega|_g}\right)^{\frac{p}{n}}, \tag{2}$$

where the subscripts g, g_0 in $|\Omega|$ indicate in which metric the volume is considered, and $A_{p,n}, B_{p,n}$ are explicit positive constants depending only on p, n. This result can be re-stated in a suitable way if we replace Ω by M, whenever M is a compact (boundaryless) manifold. Inequality (2) is not possible for $p > n$, in fact we can always find a metric $g \in [g_0]$ of fixed volume and $\lambda^g_{2,p}$ arbitrarily large. The upper bound (2) implies bounds of various types on the conformal p-eigenvalues, which we define in [1], and on eigenvalues on surfaces.

On the other hand, if we fix a metric g, we prove in [1] an upper bound of the form (1) for any $p > 1$:

$$\lambda^g_{k,p} \leq A_{p,n}\kappa^p + B_{p,n}\left(\frac{k}{|\Omega|_g}\right)^{\frac{p}{n}}, \tag{3}$$

In particular, when $M = \mathbb{R}^n$ we have $\kappa = 0$.

Another interesting behavior is shown by the *Steklov* eigenvalues $\{\sigma_{k,p}\}_{k\in\mathbb{N}}$ of the p-Laplacian on an *Euclidean* domain Ω. These are the eigenvalues of $-\Delta_p u = 0$ in Ω, $|\nabla u|^{p-2}\partial_\nu u = \sigma|u|^{p-2}u$ on $\partial\Omega$ (the unknown eigenvalue is σ). Here the interplay of the geometry of the boundary $\partial\Omega$, p and n gives raise to interesting situations. In particular in [2] we prove that, if $1 < p \leq n$

$$|\partial\Omega|^{\frac{p-1}{n-1}}\sigma_{k,p} \leq \frac{C_{p,n}}{I(\Omega)^{\frac{n-p}{n-1}}}k^{\frac{p}{n}}, \tag{4}$$

while if $p > n$

$$|\partial\Omega|^{\frac{p-1}{n-1}}\sigma_{k,p} \leq C'_{p,n}D(\Omega)^{\frac{p-n}{n-1}}k^{\frac{p-1}{n-1}}. \tag{5}$$

Here $I(\Omega)$ is the isoperimetric ratio of Ω, namely $I(\Omega) = |\partial\Omega|/|\Omega|^{\frac{n-1}{n}}$, where $|\partial\Omega|$ is the measure of $|\partial\Omega|$, and $D(\Omega)$ is what we have called the $(n-1)$-*distortion* of $\partial\Omega$, namely $D(\Omega) = \sup_{x\in\mathbb{R}^n, r>0}|\partial\Omega \cap B(x,r)|/r^{n-1}$, where $B(x,r)$ is the ball centered at x of radius r. The constants $C_{p,n}$, $C'_{p,n}$ are positive and depend only on p, n.

Bound (5) involves the constant $D(\Omega)$ which is unexpected for Steklov-type problems, in fact only $I(\Omega)$ is expected to be necessary in upper bounds, as for the case $p = 2$. However, we prove in [2] that the constant $D(\Omega)$ in (5) is necessary, and its exponent is sharp. The constant $D(\Omega)$ measures the concentration of the boundary measure in small regions of $\mathbb{R}^n$, and in the regime $p > n$ this affects the spectrum in a rather singular way, giving raise to arbitrarily large (normalized) eigenvalues. This phenomenon is new for these kinds of problems, at least to our knowledge. The bounds (4),(5) are improved under further assumptions, such as convexity, in [2].

Paper [1] has been submitted on November 2, 2020; paper [2] has been submitted on December 2, 2020. L. Provenzano is member of SBAI since October 15, 2020.

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L. Provenzano

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Spectral Geometry of Riemannian manifolds

Spectral Geometry investigates relationships between geometric structures of Riemannian manifolds and spectra of various elliptic operators. Our research in the period 2018-20 focused on the following topics:

A. Morse index and topology of self-shrinkers

B. Eigenvalue estimates under Robin boundary conditions

C. Asymptotic behaviour of eigenvalues of the Steklov problem

D. Ground state energy estimates for the magnetic Laplacian on Riemannian cylinders

A. Self-shrinkers are orientable, isometrically immersed hypersurfaces $x : \Sigma^m \to \mathbf{R}^{m+1}$ whose mean curvature vector field H satisfies the equation $X^\perp = -H$. They play an important role in the study of singularities developed along the mean curvature flow and have been extensively studied in recent years.

Now, self-shrinkers are also critical points for the functional given by the gaussian weight $\Sigma \mapsto \int_\Sigma e^{-\frac{|x|^2}{2}}dx$: they are examples of so called f-minimal hypersurfaces. As such, they possess a Morse (or stability) index (which can be viewed as the maximal dimension of a space of deformations along which the gaussian weight is decreasing) and it is of great interest to estimate it in terms of topological invariants.

A guiding principle is that if Σ has complicated topology, then it is highly unstable. To that end, for minimal hypersurfaces Σ^n of the sphere of arbitrary dimension n the author was able to show that the Morse index is bounded below by a linear function of the first Betti number $b_1(\Sigma)$ (which is the dimension of the cohomology space in degree 1), see A.Savo, Indiana U. Math. J. **59** 3, 823-837 (2010). Adapting the test-functions to the case at hand, the above method yields the following lower bound for the Morse index of a compact self-shrinker in $\mathbf{R}^{m+1}$:

$$\mathrm{Ind}(\Sigma) \geq \frac{2}{m(m+1)}b_1(\Sigma) + m + 1$$

The estimate could be generalized to the non-compact case, and it holds in terms of the dimension of the space of L^2 weighted harmonic 1-forms. See publication [1].

B. On a smooth bounded domain Ω of a Riemannian manifold (M, g) the Robin eigenvalue problem is:

$$\begin{cases} \Delta u = \lambda u\,, & \text{on } \Omega, \\ \dfrac{\partial u}{\partial N} = \sigma u & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where $\sigma \in \mathbf{R}$ is a parameter (the Robin parameter) and N is the inner unit normal. The interest in this operator is that, if $\sigma \geq 0$, it interpolates between the Neumann problem ($\sigma = 0$) and the Dirichlet problem ($\sigma \to +\infty$). The case of negative parameter is also very intriguing, and eigenfunctions show interesting properties of concentration when $\sigma \to -\infty$. The first eigenvalue $\lambda_1(\Omega, \sigma)$ models heat diffusion with absorbing ($\sigma > 0$) or radiating ($\sigma < 0$) boundary; it can also be seen as the fundamental tone of an elastically supported membrane.

When $\sigma > 0$ we give a positive, sharp lower bound of $\lambda_1(\Omega, \sigma)$ in terms of an associated one-dimensional problem depending on the geometry through a lower bound of the Ricci curvature of Ω, a lower bound of the mean curvature of $\partial\Omega$ and the inradius. When the boundary parameter is negative, the lower bound becomes an upper bound. In particular, explicit bounds for mean-convex Euclidean domains are obtained, which improve known estimates. We then prove a McKean-type inequality: for all bounded domains in the hyperbolic space of dimension n one has the bound $\lambda_1(\Omega, \sigma) \geq \frac{(n-1)^2}{4}$ provided that the boundary parameter $\sigma \geq \frac{n-1}{2}$. Asymptotics for large hyperbolic balls are also discussed. See [2].

C. Here we study the Steklov eigenvalue problem on cuboids of arbitrary dimension and prove a two-term asymptotic formula for the counting function of Steklov eigenvalues on cuboids in dimension $d \geq 3$. The first term is the classical Weyl term, which is proportional to the d-volume. The second term in the asymptotics, captures the contribution of the $(d-2)$-dimensional faces of the cuboid. The strategy of proof is similar to the one used for the Dirichlet Laplacian, the Steklov case carries additional complications. See [3].

D. We consider a Riemannian cylinder Ω endowed with a closed potential 1-form A and study the magnetic Laplacian Δ_A with magnetic Neumann boundary conditions associated with those data; under the condition that the flux of the magnetic potential around any of the two boundary components is not an integer, the first eigenvalue is positive, for which we establish a sharp lower bound and show that the equality characterizes the situation where the metric is a product. See [4].

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A. Savo

Evolution equations with memory

Contribution to the Scientific Report 2018-2020 of Department of Basic and Applied Sciences for Engineering at Sapienza University of Rome.

- **Observability inequalities.** Exponential kernels $k(t) = \beta e^{-\eta t}$, $\beta, \eta > 0$ arise in viscoelasticity theory, such as in the analysis of Maxwell fluids or Poynting -Thomson solids. In [1] we consider oscillations of square viscoelastic membranes by adding to the wave equation an integral term, which takes into account the memory and prove an inverse observability inequality. The proof employs delicate Ingham type estimates. We fix $\eta = 3\beta/2$ to study the integrodifferential equation in a square. This assumption has the double target to simplify the computation for the square and to extend to the 2-d case the results given in [2]. The analysis requires an accurate evaluation of the asymptotic behavior of the eigenvalues in the complex plane, with precise estimates for the limiting case. We study the distribution of the eigenvalues in the complex plane. Indeed, using the precise expressions of the eigenvalues, we analyze the behavior of partial gaps helpful to get the observability estimates (see Fig.1 for the dependence of eigenvalues on parameter β).

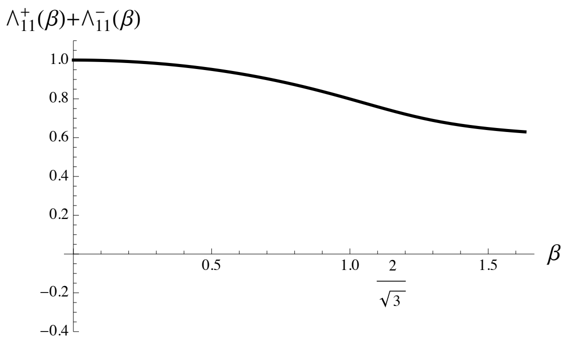

Figure 1: Plot of the function $\beta \to \Lambda^+_{11}(\beta) + \Lambda^-_{11}(\beta)$

- **Global existence and hidden regularity.** The paper [3] is devoted to prove global existence and hidden regularity results for nonlinear wave equations with an integral term of convolution type under Dirichlet boundary conditions. For general assumptions on the nonlinear term and on the integral kernel we are able to show some results about global existence of strong and mild solutions without any further smallness on the initial data. Some integral kernels satisfying the properties assumed are:
  - $a(t) = a_0 \int_t^\infty \frac{e^{-\alpha s}}{s^\beta}\, ds$,
    with $\alpha > 0$, $0 \le \beta < 1$ and $0 \le a_0 < \frac{\Gamma(1-\beta)}{\alpha^{1-\beta}}$,
  - $a(t) = \int_t^\infty (a_0 s + a_1) e^{-\alpha s}\, ds = (\frac{a_0}{\alpha} t + \frac{a_0 + \alpha a_1}{\alpha^2}) e^{-\alpha t}$,
    $\alpha > 0$, $a_0, a_1 \ge 0$, $\frac{a_0+\alpha a_1}{\alpha^2} < 1$, $\alpha a_1 - a_0 \ge 0$,
  - $a(t) = a_0 \int_t^\infty \frac{1}{(1+s)^\alpha} ds$,
    with $a_0 > 0$ such that $a(0) < 1$, $\alpha > 2$.

  We also define the trace of the normal derivative of the solution in such a way a regularity result holds. Those findings extend to integrodifferential equations with nonlinear terms well-known results available in the literature for linear wave equations with memory.

- **Reachability.** In [4] we solve the reachability problem for a coupled wave-wave system with an integro-differential term. A number of physical problems are modelized by coupled systems. The control functions act on one side of the boundary. In our case the compact perturbation method does not apply any more, even if we use two control functions. We prove the controllability by using two controls. Our method can be adapted to the case of one control function too. The estimates on the time is given in terms of the parameters of the problem and they are explicitly computed thanks to Ingham type results. Our proof yields a sufficient controllability time T_β that converges to the critical controllability time T_0 as the parameter β tends to zero. However, we cannot pass to the limit to recover the corresponding result in the case without memory, because the eigenvalues of the integro-differential operator are not bounded for $\beta \to 0^+$. It remains an open question whether the critical controllability time is independent of the parameter β (depending on the kernel). Our findings can be applied to concrete examples in viscoelasticity theory.

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D. Sforza, P. Loreti

Graceful polynomials of graphs

A *graph* $G = (V, E)$ is a collection V of v points (*vertices*) together with a collection E of e *edges* connecting some (or possibly all) pair of vertices. A graph is *graceful* if its vertices can be labelled with distinct integers in $[0, e]$ in such a way that the differences on edges cover (in absolute value) all positive integers from 1 to e. Born in the 60s of last century, gracefulness is nowadays a well established branch of graph theory; while constructions of graceful graphs are available for many infinite classes, a more difficult issue is the search of necessary conditions.

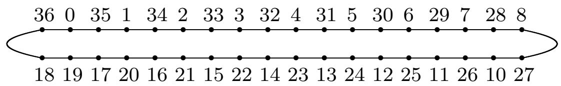

Figure 1: The 36-cycle, gracefully labelled

Graceful *trees* play a special role as in many other contexts, particularly because a now old conjecture states that all trees are graceful. Disproving this conjecture could be possible if some suitable necessary conditions for gracefulness were found.

The pioneering work on necessary conditions is [2]; in that paper, a nice interaction between algebra and combinatorics led to rule out all graphs with even degree and e congruent to 1 or 2 (mod 4). The same approach has been generalised in [3], and [4], after realising that the basic tool in [2] was the first symmetric function on edge differences, namely the polynomial

$$\mathcal{S}^1_{(G,\lambda)} \quad = \sum_{1\le i\le e} (x_i - y_i) \ ,$$

where x_i and y_i are the smaller and larger label on the i-th edge. With this in mind, the generalisation provides a family of polynomials in as many variables as the number of vertices,

$$\mathcal{S}^n_{(G,\lambda)} \quad = \sum_{1\le i_1<i_2<\ldots<i_n\le e} (x_{i_1} - y_{i_1})\cdots(x_{i_n} - y_{i_n}) \ ,$$

that becomes the so-called *graceful polynomials* once evaluated (mod 2) in order to get rid of the signs in every binomial.

In the same spirit as in [2] it was possible to explore the algebraic properties of these polynomials so as to unveil new necessary conditions related to gracefulness. The basic idea behind this development is that it is easy to evaluate the congruence class (mod 2) of any given polynomial because the binomials in the selected symmetric function are all possible integers from 1 to e, due to the hypothesis of gracefulness; after this preparatory evaluation, the contradiction with gracefulness holds whenever the expected value 1 is different from the algebraic evaluation leading to 0. This last parity follows only under precise circumstances and strongly depends on the local structure of the graph under examination. It becomes therefore crucial and not at all elementary to devise ad hoc graphs which on one hand yield an odd parity while on the other hand give rise to a graceful polynomial (of any suitable degree) that vanishes (mod 2).

The results so far obtained concern the smallest degrees up to 4 (see [4]); a promising research project concerns the fifth polynomial (see [3]) and possibly larger degrees. The main results are the following theorems.

Theorem 1. [4]

Let G be a graph having some odd vertices. The polynomial $\mathcal{S}^3_G$ vanishes (mod 2) on G precisely in one of the following two cases.

(A) G is a complete graph K_{4t+2}, for some positive integer t, possibly having $4u$ additional vertices and $4u(4t+2)$ additional edges that connect these vertices to the above complete graph.

(B) G is obtained by taking two complete graphs K_a, K_b and n additional vertices satisfying one of the following conditions: (B_1) $a \equiv b \equiv 2 \pmod 4$ and $n = 0$; (B_2) $a \equiv b \equiv n \equiv 1 \pmod 4$ with the exclusion of $a = b = n = 1$; (B_3) $a \equiv b \equiv n \equiv 3 \pmod 4$; every additional vertex must be then connected to all the vertices of K_a and K_b.

Theorem 2. [4]

Let G be a graph having at least 4 edges and some odd vertices. The polynomial $\mathcal{S}^4_G$ vanishes (mod 2) on G if and only if G is a 3-cycle together with a further edge, which can be either pendent or disjoint from the cycle.

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A. Vietri

Self-organized-criticality in sand pile models

At the turn of the eighties and nineties, a general idea surfaced in the physics literature: certain nonlinear dissipative systems drive themselves autonomously to a critical state acting as a *finite-time* attractor of the dynamics. This property is referred to as *self-organized-criticality, SOC*.

At the same time, in the early nineties, *particle models* for avalanches and sand piles provided the numerical evidence supporting the SOC finite-time property. The mechanism underlying the dynamics was described as a *toppling process* involving the particles of the pile, and the pile was supposed to consist only of a *finite number* of particles. We refer to the early papers by P.Bak, C. Tang and K. Wiesenfeld and by D. Dahr and M.Creutz , as well as to the papers by P. Bántay, I.M. Jánosi and by J.S. Carlson and G.R. Swindle who reformulated the automata models as nonlinear difference equations. In these particle models, the toppling of 4 particles at the site ij occurs only if the height of the pile at ij and at each of the four receiving sites $k\ell$ remains also supercritical.

A related sand pile problem was formulated in 2010 by V. Barbu, as a multivalued nonlinear diffusion equation in the plane. In this model, given a critical configuration $h^c(x)$, where x belongs to a bounded open domain Ω of $\mathbb{R}^2$, and set $\zeta(x,t) = h(x,t) - h^c(x)$, where $h(x,t)$ represents the height of the pile at x at the time $0 < t \leq T$, $T > 0$, the problem is formulated as

$$\begin{cases} \frac{\partial \zeta}{\partial t} - \triangle \eta = 0, \quad \eta \in \mathbf{H}(\zeta) \\ \eta \in L^2(0,T;H_0^1(\Omega)), \\ \zeta(x,0) = \zeta_0(x)\,, \end{cases} \tag{1}$$

where Δu is the Laplace operator in Ω, $\mathbf{H}$ denotes the Heaviside graph.

For this problem Barbu proves, under natural conditions, the existence of a unique solution and SOC-properties.

A stochastic version of this model was developed by V. Barbu, G. Da Prato, Rökner and, later, by Gess. A problem left open by Barbu, and co-authors is whether the initial value problem can be approximated by discrete, finite-difference particle equations. In this regard, some remarks on the numerical solutions of the PDE model can be found in that paper.

The models mentioned so far are of variational nature. Related sand pile theories, based on the notion of *angle of repose* and differential equations, were also developed by various authors, but SOC-properties have not been highlighted in the models.

It should be noticed that between the particle models and the mathematical models based on partial differential equations there is no obvious direct connection. In fact, sand piles and toppling processes are exemplary in general physical terms of large particle systems with short-range and fast-time dynamics and are intrinsically discrete in nature, contrary to the initial value problems mentioned before, which have a continuous nature and contain no toppling process overtly visible. There is thus an unexplored field between the two kinds of models.

A *purely discrete model* involving *infinitely many particles* was presented in [2]. This paper is based on the general principle that particle interactions occurring at shorter and shorter range – as in sand piles and avalanches – must be recorded at faster and faster observation times. This principle is implemented by applying a suitable *synchronization* of the time and space variables. The main achievement of this work is to obtain the SOC finite-time property in a fully discrete setting, where the limit from finitely many particles to infinitely many particle is carried out. The relevance of this result is that it shows that the finite-time property of self-organized-criticality systems has its roots – as it is in the physics literature – in particle theory and not in partial differential equations. In [2], however, no connection with PDEs is carried out. The paper [3] gives such a connection and provides a bridge between particles and PDEs, between discrete models and models in the continuum, and in this sense it is an additional contribution to the sand pile models mentioned so far. More precisely, in this paper we present a discrete sand pile model based on suitable finite-difference equations in time and space, which involves a sequence of piles composed of a finite number of particles of increasing cardinality distributed on planar uniform grids of decreasing mesh size, and we prove that the solutions of the finite-difference equations have a limit, though in a weak sense, when the number of particles tends to infinity. Moreover, the limit function is the unique solution of a nonlinear PDE. The limit from finite-differences to PDEs is carried out in coordinate Sobolev spaces.This limit is in turn related to the theory of so-called $M-$*convergence* of subspaces of a Hilbert space introduced in [1], $M-$convergence properties are summarized in the forthcoming paper: "On the external approximation of Sobolev spaces by M- convergence" (in collaboration U.Mosco).

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Integral and supremal representation in the local and nonlocal setting

Many problems in Applied Sciences are formulated as equilibria. From the applications' view point some are modelled as minimimum of integral energies, others appear as mimimum of quantities which are maximum of certain entities, and very recent theories, such as in Mechanics, appear in terms of nonlocal models.

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i) Integral representation.

In context like elasticity, plasticity, fracture mechanics, micromagnetics, etc., one has to look for minimization of suitable integral functionals. Quite often the given problem does not admit a minimum so it is important to determine, with variational tools, another functional, 'close' to the given one, whose minimum points exist and can be achieved as limits of infimizing sequences of the first functional. It is crucial then, not only guaranteeing the existence of such limiting functional but also to represent it. In particular, one of the main targets in my research consists of determining if the above mentioned integral functional, arising from equilibrium problems in the applied sciences can be seen as the restriction to open sets of a suitable Radon measure absolutely continuos with respect to a suitable given measure directly emerging from the context of applications. In particular, it is crucial to detect the density with respect such measure. This integrand, when possible, and no singularity effect comes into play (such as in 4.) can be determined by means of comparison arguments, and blow-up techniques.

The analized models come from homogenization theory, thin structures modeling and immage decomposition, see 3 and 5.

ii Supremal functionals and L^p approximation.

Some realistic problems are often min-max ones. E.g.: In chemotherapy, one minimizes the maximum tumor load. In numerical analysis, one has to find the best Lipschitz approximation to a given function (connected as well to a controlled eikonal problem).

Hence, in many context if it not important to detect averaged conditions but it is preferable to determine some maximum quantity, for instance when sets of small measure cannot be neglected. This is the scope of supremal functionals (of the type $\|f(x,u(x),\nabla u(x))\|_{L^\infty(\Omega)}$) introduced in the '60 by Aronsson, also in connection with the partial differential equations in terms of Δ_∞. In particular the "Euler-Lagrange" equation (Euler -Aronsson equation) associated with such functionals involve the Δ_∞. Necessary and sufficient conditions on f have been investigated, in order to ensure the lower semicontinuity of the functionals both in the scalar and in the vectorial case. The deep connection with constrained integral functionals are also investigated and highlighted. Finally, having in mind the approximation of the L^∞ norm by the L^p one, power law approximation has been established in 1. under suitable conditions.

iii Nonlocal supremal functionals.

In the framework of perydinamics, functional analysis, machine learning, etc: double integrals or nonlocal supremal functionals play a crucial role.

In 2. we have introduced non loocal supremal functionals of the type $\sup \mathrm{ess}_{(x,y)\in\Omega\times\Omega} W(u(x),u(y))$ with $u \in L^\infty(\Omega;\mathbb{R})$ providing necessary and sufficient conditions on the density W (the *supremand*) to ensure weak $*$ lower semicontinuity. We also made a parallel with the existing theories for nonlocal functionals in the integral setting, and extended some of the results holding in the supremal local context. This last point required a suitable generalization of some convexity properties. Finally, when there is a lack of lower semicontinuity, an explicit relaxation result has been also proven.

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E. Zappale

Research Activities: Physics

Physics - Introduction

In this brief introduction we would like to mention the scientific activity of the researchers who worked in the Physical Sciences at our department in the period 2018-2020. As already described in the previous scientific report of the period 2015-2017, all the activities have been developed according to guidelines research consolidated in the department, and framed within some specific macro-sectors of fundamental and applied physics such as *electromagnetism, classical and quantum optics, acoustics, condensed matter, plasma physics, nuclear physics, spectrometry*.

We also report an orthogonal classification based on fields of application, which helps to understand the spontaneous aggregations of researchers in the context of many active research projects, national and international collaborations with universities, industrial partner research centers and scientific consortia. Most of the research activities have therefore been focused around specific areas of applications aimed at the development and characterization of innovative materials (such as *nano-structures or meta-materials*), applications of *non-linear optics and nanoplasmonics*, a wide spectrum of *biomedical applications* (such as *bio-sensing, adrotherapy, ultrasound diagnostics*), *advanced acceleration techniques*, *energy applications, archaeometry, radiation protection*. Most of these applications require the development of new non-destructive diagnostics, based on acoustic, thermal, optical, X-ray, and nuclear detectors. Innovative computational activities are also performed, especially in the areas of plasma physics, nanomaterials and adrotherapy.

A significant part of the experimental research in Physics is led in each laboratory at SBAI by a team of researchers under the supervision of the Chief scientist (RADRL i.e. head of lab). All technical details on the instruments, setup and facilities are specifically described at the end of this report. The laboratories are always open to the Sapienza community and to external researchers for specific joint research programs. For investigations requiring larger facilities SBAI research teams made use of the national and international facilities, such as those at INFN, CNR, CINECA, CERN, GSI, and in the LaserLab consortium, according to well established collaborations.

Finally, the significant number of research contracts with industries, startups, regional, national and international institutions, which provided the department with the necessary research funding, should be noted. We cite as an example:

CHALLENGES a H2020 project that aims at developing multipurpose nano-optical techniques and metrological protocols for real-time characterization of materials.

ENSEMBLE3, a European project for the establishment of a Centre of Excellence for Nanophotonics, Advanced Materials and novel crystal growth-based technologies.

COMPACTLIGHT a European project devoted to design a hard X-ray FEL facility beyond today’s state of the art.

ATOM project (Advanced TOmography and Microscopies) funded by Lazio regional program for the establishment of an open infrastructure in the field of the characterization of materials and devices, using advanced tomography and microscopy techniques.
BIOLIGHT and TURNOFF regional projects in the field of biomedical nanophotonics.
Several strategic research projects have been co-funded by the Ministry of Defense in the framework of the PNMR program (SCHERMA, COPERNICO, STORM) establishing a consolidated and continuous partnership among Sapienza, the Ministry of Defense and industries.
Research on plasma physics, for applications to the fusion and acceleration of particles, has been carried out continuously within European projects (HiPER, Eurofusion ER), in collaboration with US universities and laboratories, and with INFN.
At the same time several research activities in cultural heritage, biology and medicine, particularly strategic for the SBAI department have been activated and co-funded.
In conclusions we are all very grateful to the scientists who contributed with their enthusiasm, efforts, will and determination (be free to choose your favorite order!) to the research excellence of the department, always keeping in mind the Sapienza motto "*the future is passing through here*".

Laser-driven intertial confinement fusion and high energy density plasma phsyics

Research on thermonuclear fusion aims at the development of a practically inexhaustible energy source, with low environmental impact, based on fusion reactions between the isotopes deuterium (D) and tritium (T) of hydrogen. One approach to fusion is based on laser-induced inertial confinement (ICF). In ICF, a cryogenic DT target is imploded to high density and temperature using direct laser light illumination or laser-generated thermal x-rays. The fuel is ignited from a central hot spot generated at implosion stagnation. After the first demonstration of hot spot self-heating in 2014, current research focuses on the physics of burning plasmas and on the study of robust concepts suitable for energy production.

In 2018-2020 SBAI plasma physics group participated in several projects in the fields of ICF and basic high energy density plasma physics (HEDP). Such activities were performed in the frame of i) a Eurofusion project on the ICF scheme of Shock Ignition; ii) a collaboration with MIT Plasma Fusion center; iii) a collaboration with Ecole Polytechnique; iv) experiments supported by the EU LaserLab programme. The main activities can be summarized as follows

Shock ignition target studies. In the shock ignition ICF scheme, a first laser pulse drives target implosion, and a second, shorter and more intense pulse generates a strong shock wave, with pressure of 200–400 Mbar, contributing to hot spot creation. Our previous studies led to the definition of a reference target for ignition experiments. A crucial issue is the design of concepts with sufficiently large 1-D safety margins, capable of tolerating unavoidable departures from design specifications. We then used 2-D simulations with our radiation-hydro-nuclear code DUED to investigate the effects of low- to intermediate-mode (modes $l = 1$–8) implosion asymmetries [1]. It turned out that modes $l = 2$–4 are the most damaging ones (Fig. 1). We found a relation between allowed perturbations and the 1-D safety margin, and suggested ways to increase such a margin.

Experiments on laser-plasma interaction and laser-induced shock-waves. We participated in the design and interpretation of two classes of experiments. i) Experiments (conducted at the LLE-Rochester OMEGA laser, and Prague PALS laser) on laser-plasma interaction under conditions relevant to shock ignition, i.e., laser intensity larger than 5×10^{15} W/cm^2, plasma temperature higher than 2 keV, and relatively long plasma density scale-lengths. The fraction of laser energy converted into hot electrons by parametric instabilities (in particular Raman back-scattering) was measured [2,3]. It was also shown that such hot electrons should not damage compression of the fusion fuel [2]. ii) Laser-driven implosions of gas-filled thin glass-shells (conducted at OMEGA by a collaboration led by the MIT group): for the first time, evidence was found for ion-species separation caused by the propagation of a strong shock wave in the low density inner gas [4]. We contributed with systematic simulations with DUED.

Proof-of-principle of phase-contrast imaging of laser-driven shock-waves. In 2017, a collaboration lead by L. Antonelli (then in our group) proposed and performed (at GSI PHELIX laser) a proof-of-principle experiment on the use of phase-contrast radiography for the diagnosis of plasmas compressed by strong shock waves. Analysis of the acquired data, performed in 2018 clearly showed that this technique can unveil features not detected by conventional absorption radiography [5]. Synthetic phase-contrast radiography (using DUED simulation results as an input) was specifically developed in order to compare experimental data with simulations.

Simulation code upgrades An extended magneto-hydrodynamic package is being introduced in the DUED code. It accounts for magnetic field evolution and its effects on plasma dynamics and transport. A package for ion viscosity was also introduced in the 2D Cartesian version of the code.

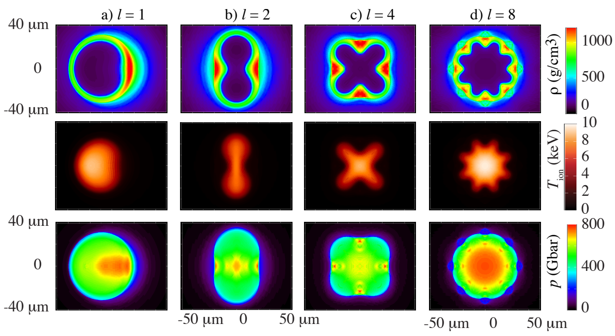

Figure 1: 2-D simulation of a shock ignition target. Maps of density, ion temperature and pressure at the instant of hot spot formation are shown for cases with velocity perturbations described by a single mode ($l = 1, 2, 4, 8$, respectively), with the same initial amplitude. The largest hot spot deformations occur for $l = 2$ and $l = 4$.

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http://gaps.ing2.uniroma1.it

Chiral plasmonics and photonics: linear and nonlinear circular dichroism of nanostructured metasurfaces

Taming chiral light at nanoscale is of importance for optical molecular sensors. Indeed, natural molecules are typical chiral objects and absorb circular polarised light in different amount for right or left handed polarisation. But, due to the small dimensions of the molecules typical absorption band lies in the UV region of spectrum. Plasmonic nanostructured materials give the opportunity to confining visible and NIR light into nanometric dimensions so that to squeeze longer wavelength light into to dimensions of molecules and increasing the reciprocal interaction. Thus, plasmonic nanostructured chiral surfaces can be used to enhance the recognition of chiral molecules. In order to obtain a large area surface with chiral nanostructures, bottom-up self-assembled approach offer interesting and feasible solutions. Different techniques can be adopted to characterise chiral nanostructures and retrieve the circular dichroism (CD). In [1] we compared the CD measured by optical reflectance (OR), photo acoustic absorbance (PA) and second harmonic generation (SHG) [2]. Here we show measurement of CD on self-organized samples by using extinction spectroscopy in transmission (EST) and by photo acoustic absorbance. The samples were realised starting by polystyrene spheres (518nm) deposited on glass substrate to produce asymmetric hole array on a metal thin film.

The spheres where reduced by selective reactive ion etching and then covered by 30 nm of different metals, Au, Ag, Cr, that are evaporated at a glancing angle, realising three samples. A fourth sample was obtained after the removing of the spheres from the Au sample. They present elliptical-hole array in the metallic layer.

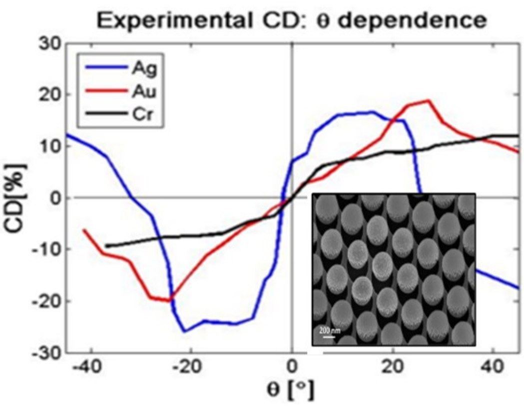

Figure 1. Measurement of optical CD at 633nm for the first generation samples by photo-acoustic technique; In the inset the SEM image of the realised sample.

The asymmetric distribution of metal due to glancing angle deposition both in the first generation samples and in the second generation ones leads to a strong circular dichroic behaviour. The measurements on fig.1 where obtained by mean of PA technique [3], while the ones on fig.2 by means of EST [4]. The CD response of light interacting with the substrate can be tuned by choosing proper incidence angle and excitation wavelength.

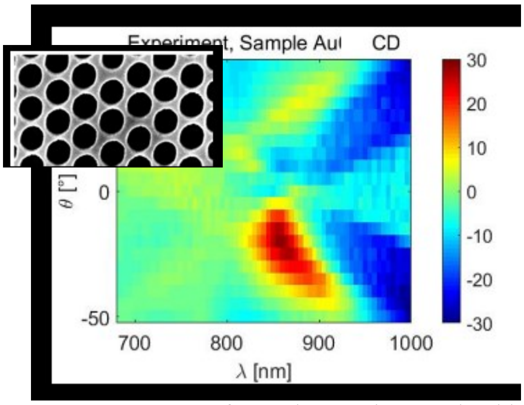

Figure 2. Measurements of second generation sample with Au metal by extinction spectroscopy. In the inset the SEM image of the realised sample.

The obtained results are very promising and show that self-assembly nano 'lithography' can lead to low-cost fabrication of high quality plasmonic samples, with large area. The chiral effects, due to intrinsic as well extrinsic chirality can be measured by means of different spectroscopic techniques as photoacoustic or extinction spectroscopy in transmission. The fabricated samples can be the first steps on compact chiral sensors for optical molecular recognition.

Part of the activity was performed in the frame of LASAFEM Sapienza Università di Roma Infrastructure Project prot. n. MA31715C8215A268.

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A. Belardini, E. Petronijevic, G. Leahu, R. Li Voti, C. Sibilia

https://www.sbai.uniroma1.it/node/7771

Biomedical and biological applications of ultrasound

Lipid-coated microbubbles (mean diameter from $\simeq 2$ to $\simeq 5\,\mu$m) filled with low diffusivity gases, are nowadays used to enhance ultrasound contrast of perfused vessels and tissues thanks to the great acoustic mismatch between the microbubbles and the surrounding medium. The clinical utility of dispersed solutions of gas-filled lipid-coated microbubbles – also known as ultrasound contrast agents (UCAs) – has been established in applications spanning cardiology and radiology The attenuation of ultrasound (that is the sum of absorption and scatter) caused by dispersed solutions of microbubbles, is an important physical parameter to be measured for improving and optimizing their backscatter properties. The increase in the ultrasonic frequencies used in diagnostic ultrasound scanning systems, causes a new generation of UCAs to be engineered, by reducing the bubble diameter, so to resonate when irradiated with high frequencies acoustic waves (> 10 MHz); consequently, a new generation of UCAs is being studied made of liquid solutions of nanobubbles (mean diameter $\simeq 100$ nm). Furthermore, the elastic characteristics of lipid-coated microbubbles and nanobubbles are becoming even more important to be measured as these systems have been recently promoted for transport and delivery of various bioactive substances, thus providing a technique for non-invasive gene therapy and drug delivery.

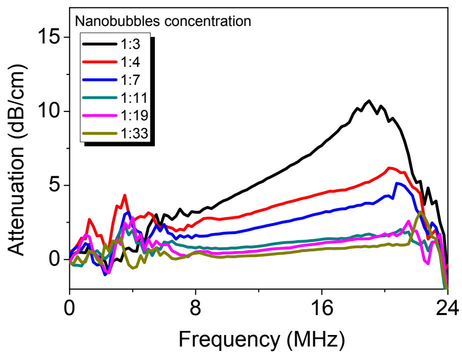

Figure 1: Acoustic attenuation spectra of lipid-coated nanobubbles as function of nanobubbles concentration

In our research a high-frequency broadband ultrasonic pulse-echo measuring technique is employed for nondestructive evaluation of temperature and frequency dependence of the backscatter coefficient of lipid-coated microbubbles and nanobubbles. A new generation of gas-filled nanobubbles is currently under development in collaboration with the Department of Chemistry and Technology of Drugs at Sapienza University, to be used as a ultrasound contrast agent in ultrasound scan of vascular systems with small and very small vessels diameter and in small animals ultrasonography.

The demand for *in situ* surface analysis systems has greatly increased in recent years due to the development of nanotechnologies. In the biological field, in particular, there is an increasing interest in the creation of biosensors that are simple from a constructive point of view and support electronics and that, at the same time, allow a rapid, selective, but non-specific, measure and control of biological events occurring under particular conditions. Acoustic waves devices with shear displacements such as quartz crystal microbalance (QCM) and high frequency shear horizontal acoustic wave devices provide sensitive probes that meet the requirements described above and, consequently, they are increasingly used in the biological field.

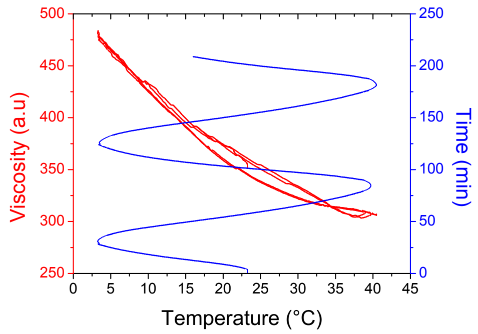

Figure 2: Viscosity of red blood cells measured through QCM-based biosensor as function of periodically varying temperature

We are currently working on a QCM-based biosensor for the real-time study of cell-substrate interactions and for the measurement of the fundamental viscoelastic properties of biological fluids under controlled frequency, stress, strain, shear rate, time, and temperature. In particular, we have focussed our research on blood viscoelasticity because, a good understanding of the hemodynamics through the main vessels of the human circulatory system is fundamental in the detection and in the treatment of cardiovascular diseases.

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Hybrid Yagi-Uda Nanoantenna Design for Tailored Infrared Thermal Radiation

The availability of low cost, integrated, radiation sources in the infrared with a narrow-band emission spectrum is of great importance in a variety of applications such as infrared sensing, thermophotovoltaics, radiation cooling, and thermal circuits [1]. An easy way to obtain infrared radiation is to take advantage of thermal emission form a heated body. However, the spectral and directional control of thermal emission is a challenging task due to the incoherent behavior (both spatially and temporally) of the thermal radiation. In the optical and near infrared ranges remarkable results have been obtained by using Yagi-Uda nanoantennas coupled with quantum dots emitters [2]. The Yagi-Uda design consist on a feeder which plays the role of the emitter, a mirror which is used to suppress backward radiation and a set of directors which are responsible for the directivity of the emission pattern (see inset of figure 1. In a typical Yagi-Uda antenna, the enhanced directionality and backward suppression are achieved by proper control of destructive and constructive interference between emitted and scattered waves. However, thermal radiation originating from chaotic fluctuations is responsible for highly incoherent signals which dramatically reduce the effect of interference due to the lack of coherence. For this reason, in order to tailor the far field emission pattern of a thermal nanoantenna, we numerically studied the near field interaction between different elements and the multipolar emission of all the device rather than considering the interference between propagating and scattered waves from each element.

As a starting point we considered SiC dipole antennas as feeders, operating at 400 K. The length and section of the rods have between designed in order to have a single resonance in the wavelength range around 12 μm. Because of the high emissivity of the SiC due to the excitation of phonon polaritons it is possible to select a narrow emission line by properly tailor the length and the thickness of the SiC rods. We used Au elements to work as the mirror and the directors' elements. The numerical study was performed by modifying a previously developed model based on the fluctuational electrodynamics approach and on the discretization of the resulting volume integral equation to calculate relative emissivity and spatial emission pattern of nanoparticle ensembles [4]. In figure 1 we report the emission pattern of an optimized 2-director antenna at its resonant wavelength of 12 microns. We show that despite of the chaotic nature of thermal radiation it is possible to obtain efficient highly directional and narrow bandwidth antennas in the mid to far IR by adapting the Yagi-Uda scheme with a combination of metallic and polar materials. Our calculations show that it is possible to tune the emission wavelength by properly choosing the resonance of the feeder. We compare the performances obtained with hybrid antennas with respect to all metallic antennas and discuss how to improve specific features for different kind of applications.

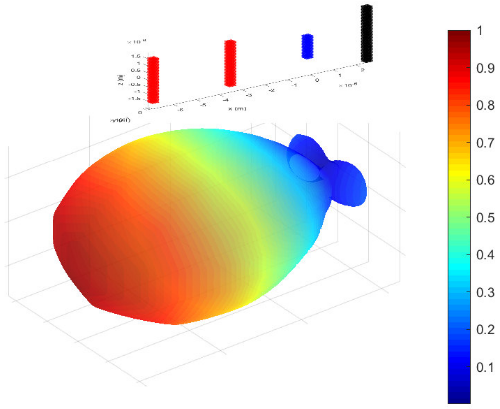

Fig. 1. Normalized emission pattern at the resonance wavelength of 12 microns of a thermal Yagi-Uda antenna composed of two directors. In the inset the scheme of the antenna: mirror (black), feeder (blue) and two directors (red).

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Authors

M. Centini, M. C. Larciprete, R. Li Voti, C. Sibilia

Optical Artificial Intelligence: Solitonic Neurons able to perform both Supervised and Unsupervised Machine Learning

Photorefractive Spatial Solitons are specific states of the nonlinear propagation of light beams which, by modifying the refractive index of the host material, compensate for the natural diffraction. As a result, self-confined light beams are obtained in channels of increased refractive index. These channels can be used as solitonic waveguides from other signals. In this way it is possible to build transient circuits, which are written and erased as needed. Not only that: the solitonic waveguides are perfectly addressable as they are not static but dynamic structures. They can be written and addressed by making them reflect or refract on electrical interfaces (fig.1), i.e. on interfaces created by applying abrupt electric gradients [1-2].

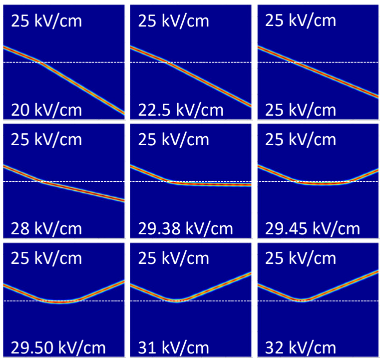

Figure 1. Refraction or total reflection of solitonic waveguides on electric interfaces.

Solitonic waveguides can also be used to perform logical machine learning operations. By crossing two solitonic waveguides to form an X-junction, both supervised machine learning [3-4] and unsupervised machine learning [5] processes can be implemented. Supervised learning was implemented by unbalancing the intensities of the soliton beams that wrote the channels of the X-junction: the information carried in the junction is always directed towards the more intense output channel [3]. This process can also be exploited to realize unsupervised learning, allowing the information signals transported to modify in turn the refractive index of the soliton channels. In this way, reinforcement learning is obtained through the modification of the propagation structures by the signals. This form of communication through the modification of the surrounding environment takes the name of STIGMERGY and is typical of animal colonies, which are able to carry out complex reasoning through the application of many elementary decision-making processes (complex reasoning through a distributed intelligence).

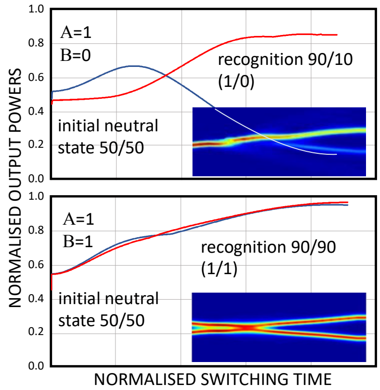

Figure 2. An X-junction is able to recognise an input state of signals and readdress accordingly.

X-junctions behave like optical neurons and can also form complex neuromorphic networks [6], capable of storing information and processing it later.

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Non-destructive analyses and archaeometry

The research activity has mainly concerned archaeometric studies of several typologies of Cultural Heritages. Archaeometry is an interdisciplinary research field in which artworks are studied not only from the humanistic point of view but also by using scientific methodologies.

Other research activities have been related to the non-destructive analysis of nanomaterials and biological samples.

The activity can be summarized in the following research lines:

Characterization of pictorial materials

Characterization of alizarin-based commercial lakes [1]. The chemical composition and the optical features of fifteen alizarin-based commercial lakes were investigated by a multi-analytical technique approach combining different spectroscopic methods and HPLC-PDA. The results obtained by UV induced fluorescence spectroscopy showed that, although it is commonly assumed that the madder lake presents an orange-pink fluorescence, the inorganic compounds, added to the recipe could induce a quenching phenomenon or an inhibition of the fluorescence.

Characterization of pigments and colorants realized following ancient recipes. By using several non-destructive techniques pigments and colorants realized following ancient recipes were analyzed. The painting materials were supplied by the Montefiascone Conservation Project during the class “Re-creating the Medieval palette”, in July 2017. The results of the analyses constitute a database for the identification of the materials used in Medieval illuminations.

Diagnostic studies of painted artworks

Vincenzo Pasqualoni's wall paintings in the apse of S. Nicola in Carcere (Rome) [2]. The wall paintings were analyzed by Multispectral Imaging. The research was part of a diagnostic study performed by several research groups in the frame of the project “ADAMO “ founded by Regione Lazio.

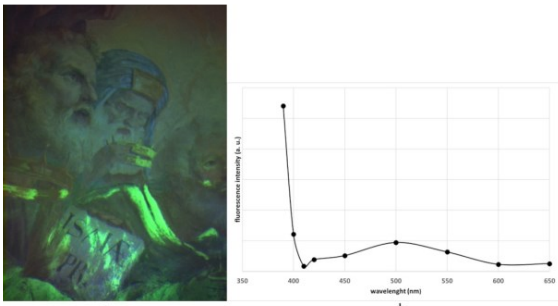
The multispectral images allowed to identify and map the presence of some pigments. In Fig. 1a it is shown a reconstructed RGB color image obtained by using UV induced fluorescence. The fluorescence emission spectrum corresponding to one of these areas reconstructed from the multispectral images (Fig 1b) shows the typical behavior of the fluorescence emitted by zinc white, confirming the presence of this pigment.

Digital restoration of manuscripts

Using ultraviolet radiation and collecting the images in different spectral ranges the readability of the text is enhanced while illuminating the manuscript with visible and infrared light and collecting the images at long wavelengths the hiding effect of spots covering the text is attenuated [3].

Archaeometric study of archaeological samples

Ancient Roman orichalcum coins [4]. A collection of ancient Roman orichalcum coins, i.e., a copper-zinc alloy, minted under the reigns from Caesar to Domitianus, have been characterized using scanning electron microscopy (SEM-EDS) and electron microprobe analysis (EMPA). Coins emitted by Romans after the reforms of Augustus (23 B.C.) and Nero (63–64 A.D) were studied for the first time. The results revealed that the coins are characterized by porous external layers, which are affected by dezincification and decuprification processes. The composition of the un-corroded nucleus is a Cu-Zn alloy containing up to 30% of Zn, typical of coins produced via cementation process.



a b

Figure 1. a) reconstructed color image obtained by using UV induced fluorescence images at 650 nm (red channel), 550 nm (green channel) and 450 nm (blue channel). b) Fluorescence emission spectrum reconstructed from the multispectral images

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https://www.sbai.uniroma1.it/node/5886

Polar Metamaterials for Infrared Radiation Managing.

Advances in nanophotonics have led to an extreme devices miniaturization thanks to the exploitation of surface plasmon polaritons (SPPs) in the visible range. Recently, different strategies have been proposed to extend SPPs in the 2-8 micron range with doped semiconductors or in graphene. Moving toward the 8−20 micron range, where vibrational absorption provides relevant information on molecular bonds and insights into protein orientation and conformation, the SPP approach proves to be less effective due to the poor field confinement at longer wavelengths. Moreover, for the development of a complete IR photonic platform, miniaturization and integration of optical components with the chip-scale platforms using facile fabrication techniques is still an open task. Several works reported on the great potential of polar materials for IR sensing applications up to terahertz (THz) regime [1] and for the realization of compact IR photonic devices. Beside their strong anisotropy related to the coupling of the electromagnetic field with lattice vibrations (phonons) they allow strong field localization by the excitation of surface waves called surface phonon polaritons (SPhPs).

We developed a metamaterial approach based on the random nanostructuration of a polar film with subwavelength dielectric elements (i.e. air ellipsoidal inclusions) for managing and leveraging SPhP through the deployment of a completely new family of modeling techniques, based on highly innovative extensions of the classical homogenization techniques such as Maxwell Garnett theory, in combination with transfer matrix method for layered structures, finite difference time domain (FDTD calculations) as well as percolative systems. The resulting theoretical model was employed to describe the infrared (IR) emissivity of several different systems with specifically tuned emissive properties. We showed that a graded air inclusion pattern into a silicon carbide (SiC) layer, only few microns thick, allows to get strong asymmetry between forward and backward emission along the normal direction to the film surface [2]. We investigated a dispersion of randomly oriented carbon nanotubes into a poly(ethylene terephthalate) matrix fibers to get polymeric yarns with both high IR emission and large electrical conduction [3]. Furthermore, we studied the possibility to get nanostructured polar materials where the conditions of surface modes hybridization can be fulfilled would allow energy transfer from nonradiating to radiating modes.

Increased versatility, to tame the IR emissivity, can be obtained by through application of an external stimuli (temperature). We thus investigated the IR emission from a thin film of vanadium dioxide (VO_2), a polar, thermochromic material which undergoes insulator to metal phase transition at a temperature of 68°C [4-5]. Experimental results revealed that the VO_2 film behaves as a metamaterial for a temperature range close to its transition temperature. The strong dynamic tuning of IR emission obtained from a single VO_2 thin film on sapphire substrate demonstrate that such thin films are promising candidates to control the thermal radiation of an underlying hot body with completely different emissivity features, i.e. a black body-like and a mirror-like heated body [4].

These achievements and further experimental investigation on polaritonic materials and structures will contribute bridging the wavelength boundaries of plasmonics. Overcoming the limit of significant losses typical of metals and doped semiconductors opens to potential outcomes in a new class of tunable and integrated IR devices.

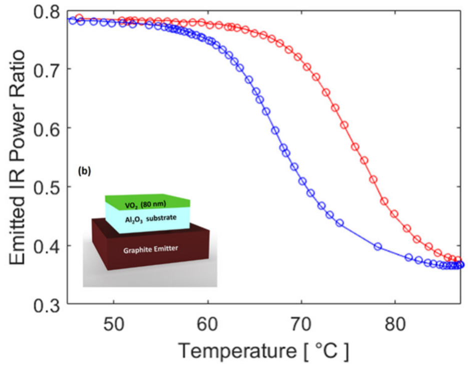

Fig. 1. Relative emitted power of the VO_2(80nm)/ sapphire/graphite system measured via IR thermography technique in the 3.3-5.1 µm wavelength range.

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Authors

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Optical and thermal characterization of metamaterials by Photoacoustic and Photothermal Techniques

One of the most challenging problems in nanomaterials research is their accurate characterization, which is fundamental for the efficient use of these technologically promising materials. Absolute absorption, quantum efficiency, thermal diffusivity, and the elastic constants are important parameters for photonic applications. Although the conventional absorption or emission techniques can provide the absorption coefficient, the determination of the absolute absorption is not a trivial measurement due to the presence of scattered light. On the contrary Photoacoustic (PAS) and Photothermal Spectroscopy are very sensitive techniques, immune to scattered or reflected light, and easy to be used to measure the absolute absorption in many different wavelength ranges. Since 1990 *Photoacoustic and Photothermal laboratory* (PA&PT lab) has been working to develop innovative instruments for optical and thermal characterization of materials [1]. In this summary we underline the advances in the PAS methodology and the new applications developed in the period 2018-2020. PAS was used to measure circular dichroism of pseudo-chiral metasurfaces [2], as well as the resonant absorption peaks related to the guided modes of GaAs-based NW on Si in the VIS/IR range [3]. In disordered media PAS was used to determine separately both the absorption and the scattering spectra allowing to estimate the size of either metallic (AgNP) or semiconductor nanospheres (ZnO) [4] (see Fig.1), as well as clusters of nanospheres bridged by the ligands.

In the framework of the project Horizon 2020 "*ENSAMBLE3*" PAS was also used to measure the band gap and the thermal properties of anisotropic materials, i.e. ZnO–$ZnWO_4$ Eutectic Composites

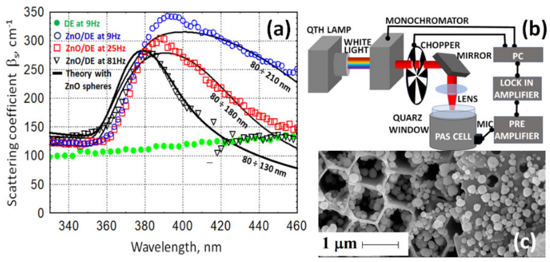

Figure 1: (a) Spectrum of the scattering coefficients measured by PAS of diatomite frustules decorated by ZnO nanospheres (80-210 nm); (b) PAS schematic sketch; (c) SEM image.

fabricated by the Centre of Excellence for nanophotonics, advanced materials and novel crystal growth-based technologies in Poland [5].

In the PNMR project "*SCHERMA*" a dedicated photothermal radiometry (PTR) and infrared thermography setup have been developed to measure the emissivity changes with temperature and the hysteresis loop in both SWIR (3-5 μm) and LWIR (8-12 μm) ranges [6-8] in VO_2 nanolayered samples deposited either on sapphire or silicon (Fig.2).

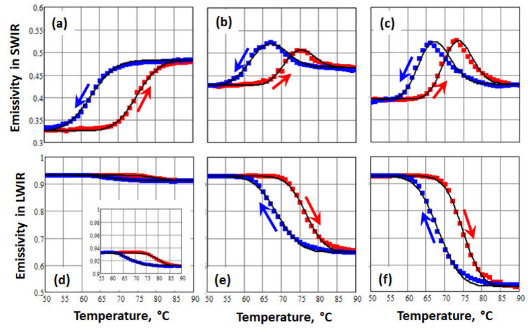

Figure 2: Emissivity vs temperature of VO_2 film deposited on sapphire by PLD in both SWIR and LWIR ranges: (a,d) 45 nm film; (b,e) 90 nm film; (c,f) 135 nm film.

Numerical models and genetic algorithms have been also developed to design nanoantennas, metasurfaces and nanolayers so to obtain directional and wavelength dependent emittance properties [9, 10]. to be integrated on flexible substrates and/or smart textiles [11].

These research topics have been developed in collaboration with CNR, ENEA, University of Padova, Ensamble3, and Tampere University of Technology.

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R. Li Voti, G. Leahu, G. Cesarini, A. Belardini, E. Petronijevic, M. Centini, M. C. Larciprete, C. Sibilia

Fluorescence emission in photonic crystal structures: application to optical biosensing and organic light emitting diodes

The theoretical and experimental investigation of the fluorescence emission of organic molecules and quantum dots embedded in or in close proximity to a resonant photonic structure (Figure 1) is of extreme relevance for applications in quantum information technologies, single molecule microscopy, fluorescence based optical biosensing techniques and fabrication of more efficient organic light emission diodes (OLED). *In collaboration with Regina Elena National Cancer Institute (IT), Fraunhofer IOF (DE).*

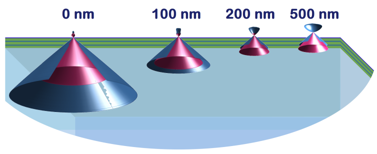

Figure 1: Angular distribution of the fluorescence emission of an ensemble of isotropically oriented molecules as a function of the distance from a 1DPC, for the TE (blue) and TM(red) polarizations.

As a first example [1-3], we addressed the fluorescence emission and photobleaching (PB) of dye molecules bound at the surface of one-dimensional photonic crystals (1DPC). We analyzed the effect of anisotropic PB on the reliability of fluorescence based 1DPC biosensors and the possibility to exploit it to probe the orientation of the emitters. Usually, in both PC- and 1DPC-enhanced stationary fluorescence, the orientational distribution of the emitters is assumed to be isotropic, even if the excitation is polarized, based on the assumption that fluorescence depolarization always dominates. However, for emitters bound at a surface (Figure 2), as for most of PC or 1DPC fluorescence biosensors, such an assumption could be wrong because rotational motion might be hindered.

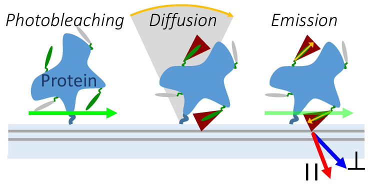

Figure 2: Scheme used for the detection of bound proteins' rotational diffusion exploiting 1DPC enhance anisotropic PB.

A significant portion of the emission of a fluorescently labeled protein in proximity of a 1DPC can couple to the available modes, either TE or TM, owing to the large local density of optical states (LDOS) provided by the 1DPC. Detecting the relative intensities of the TE and TM components can therefore permit to trace back to the emitters/proteins' orientation and eventually to their kinetics under non-equilibrium conditions, as shown in Figure 3.

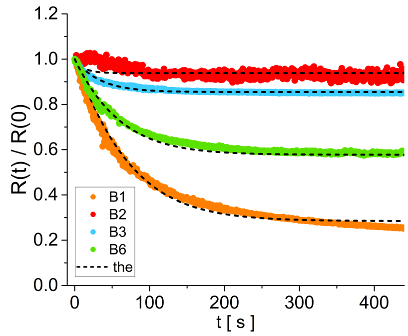

Figure 3: Anisotropic emission ratio under PB conditions for fluorescent labeled antibodies at the surface of a 1DPC. B1 to B2, from free to most tightly bound antibodies.

As a second example [4], we used the same approach to study light emission from the Rubrene derivative in a 2,4,6-tris(biphenyl-3-yl)-1,3,5-triazine (T2T) host used for the fabrication of optimized organic light-emitting diodes. Purposely tailored thin film stacks sustaining surface waves were used to create a unique link between emission angle and wavelength of fluorescent dye molecules. The knowledge of the thin film stack's properties allowed us to derive the intrinsically emitted luminescence spectrum as well as to gain information about the orientation of fluorophores from angularly resolved experiments. This corresponds to replacing all the equipment necessary for polarized spectroscopy with a single smart thin film stack, potentially enabling single shot analyses in the future. The findings illustrate how resonant layered stacks can be applied to integrated spectroscopic analyses.

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https://www.sbai.uniroma1.it/strutture/molecular-photonics-laboratory

Advanced Nano-Photonic Biosensors

Characterizing the interaction of biomolecules with bio-active surfaces in real time is of high relevance to understand the structural and functional properties of biomaterials. Indeed, the study of the interaction of proteins with other biomolecules at surfaces can be relevant for both the conception of multimolecule coatings and the in vitro assessment of the biological performance of advanced diagnostic devices for medical applications.

As a first example, the Molecular Photonics Group (MPG) developed, at SBAI Dept., a combined label-free and fluorescence surface optical technique that was used to quantify the surface coverage of binary biomolecular coatings for prosthesis implantation. These coatings were constituted by fibronectin (FN), to stimulate endothelialization, and phosphorylcholine (PRC), for its hemocompatibility, which are two properties of relevance for cardiovascular applications. One-dimensional photonic crystals sustaining Bloch surface waves (BSW) were used to characterize different FN/PRC coatings deposited by a combination of adsorption and grafting processes [1]. *In collaboration with IFAC CNR (IT) and Laval University (CA).*

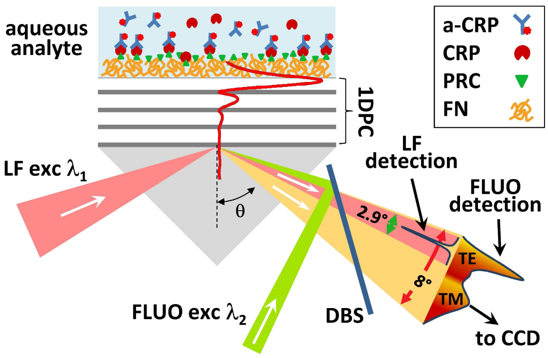

Figure 1: Simplified read-out configuration.

In the label-free operation mode the excitation of a BSW under total internal reflection conditions produces a dip in the angular reflectance spectrum; by tracking the resonance angle, it is possible to monitor changes of the refractive index with a 100nm vertical resolution as well as biomolecular interactions at the surface. Moreover, an enhanced fluorescence operation mode offers the possibility to confirm the validate the protein levels with a sharp improvement of the sensitivity and limit of detection (LoD) [2].

Performing an effective step from qualitative to quantitative biology requires new innovative approaches and close interdisciplinary collaboration among biologists, physicists, engineers, mathematicians, chemists, and computer scientists. Based on such a concept, as a second example, the MPG developed an optical biosensing platform that is able to detect cancer biomarkers using the tandem approach exploiting both label-free and fluorescence detection [3]. In particular, BSW supported by one dimensional photonic crystal were exploited to enhance and redirect the fluorescence arising from a sandwich immunoassay that involves the target biomarker. The sensing units consist of disposable and low-cost plastic biochips coated with the photonic crystal. The biosensing platform was demonstrated to detect several biomarkers (ERBB2, Ang-1, Ang-2, VEGF) in cell lysates and human plasma samples at the clinically relevant concentrations.

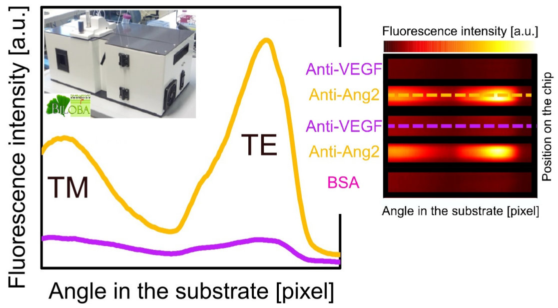

Figure 2: Ang2 colorectal cancer biomarker detection assay. Difference of the fluorescence intensities along the detection (yellow) and reference (violet) spots shown in the real-time CCD camera image.

The LoD of the platform is in the range of 0.3-2.5 ng/mL for different biomarkers pushing the platform towards the pre-clinical environment. Furthermore, the system is capable of assessing extremely low biomarker concentrations in complex biological media using small sample volumes with a short experimental time (30-45 minutes) and without sample pretreatment or dilution [4]. *In collaboration with Regina Elena National Cancer Institute (IT), Candiolo Cancer Center (IT), Politecnico di Torino (IT) Fraunhofer IOF and IWS (DE), Imperial College (UK).*

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Beam dynamics and instabilities in future accelerators

March 1, 2022

The European Organization for the Nuclear Research (CERN), among the world's largest centres for scientific research, is currently fully involved in the update of its main accelerator, the Large Hadron Collider (LHC). This ambitious program is called High-Luminosity Large Hadron Collider (HL-LHC), and it aims to improve the performance of the LHC in order to increase the luminosity by a factor of 10 beyond the LHC's design value. In order to reach such high values, an increase of the beam current, as well as the energy, is foreseen.

Due to the very long time required to build such sophisticated machines, which belong to the most complex devices that mankind has ever built, and which necessitate competences from almost every field of engineering (vacuum systems, RF, magnets, control systems, diagnostics, electromagnetism, cryogenics, . . .), of computer modeling (CAD) and software development, and of particle physics, CERN started an exploratory study for a future long-term project centred on a new generation of circular colliders with a circumference of about 100 kilometres called Future Circular Collider (FCC).

The FCC study is a global venture for particle physics and stems from the recommendation in the European Strategy for Particle Physics, published in May 2013, that a feasibility study be conducted on future fundamental research projects at CERN. The project comprises, in the same $\simeq$ 100 km tunnel, a hadron collider with unprecedented energies in the region of 100 TeV (FCC-hh), and a high-luminosity e+e- collider (FCC-ee).

In Fig. 1 a schematic map shows where the Future Circular Collider tunnel is proposed to be located in the Geneva area.

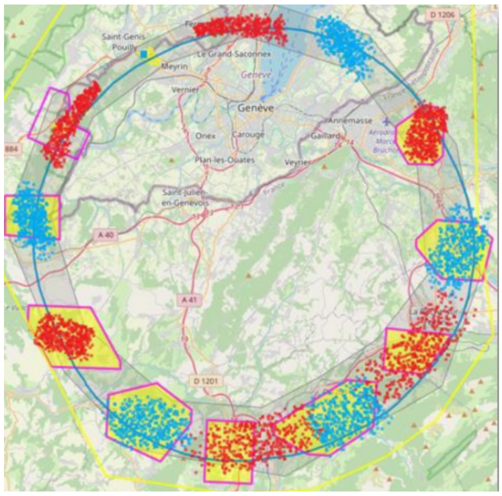

Figure 1: A schematic map showing the FCC tunnel in the Geneva area. On the top centre of the figure the Geneva town and the lake are visible.

In these accelerators the charges are guided through the design orbit and are focused thanks to magnetic fields of dipoles and quadrupoles respectively. Moreover, higher order magnets are employed for other purposes and electric fields in RF cavities are used to provide energy to the beams. In addition to these external fields which amplitude can be controlled by changing, for example, the current in the magnets or the power feeding the cavities, there is another important source of electromagnetic fields, the beam itself, which, interacting with the surrounding environment, perturbs the external guiding fields and could lead to instabilities thus compromising the performance of these machines. In particular, future accelerators as HL-LHC and FCC require beams of high intensity which could generate strong electromagnetic fields that are called wakefields.

Therefore, the study of the beam dynamics under the effects of these self induced electromagnetic fields is extremely important since they could represent one of the major limitations determining the ultimate machine performance of future accelerators.

In the years 2018-2020 our group has been collaborating with CERN on the determination of wakefields and on the study of instabilities related to the upgrade program of LHC and its injectors chain and is responsible of the work on collective effects for the e+e- collider FCC-ee [1].

In particular, for FCC-ee, we have developed a model of the accelerator taking into account the main sources of wakefields, and we have found important instabilities that could limit the maximum current stored in the machine. Therefore, many critical machine components have been analysed from the electromagnetic point of view, and an important work of optimisation, to reduce their impact on the beam dynamics, has been performed [2].

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Authors M. Migliorati, L. Palumbo, D. De Arcangelis, A. Mostacci.

Plasma Wakefield Accelerators for high brightness beams

March 5, 2022

The theoretical and experimental activity aims at the acceleration, manipulation and transport of high brightness electron beams by resonant plasma wakefields; it is conducted within a tight scientific collaboration with the Laboratori Nazionali di Frascati (INFN).

A train of high brightness bunches with THz repetition rate, so-called comb beam, is properly generated at the cathode, and manipulated through the velocity bunching technique, in order to be injected in a H_2-filled plasma discharge capillary. A train of driver bunches separated by a plasma wavelength (≈1 ps), resonantly excites a plasma wake, which accelerates a trailing witness bunch injected at the accelerating phase.

The development of compact accelerators providing high-brightness beams is one of the most challenging tasks in the field of next-generation cost affordable particle accelerators, to be used in many fields for industrial, medical, and research applications. In this regards, plasma wakefields can be also used to tune the longitudinal phase space of a high-brightness beam. Indeed, the electron beam passing through the plasma drives large wakefields that are used to manipulate the time-energy correlation of particles along the beam itself. We have experimentally demonstrated at SPARC_LAB that such a solution is highly tunable by simply adjusting the density of the plasma and can be used to imprint or remove any correlation onto the beam. This is a fundamental requirement when dealing with largely time-energy correlated beams coming from future plasma accelerators.

Furthermore, going towards compact facilities, also plasma-based focusing devices deserve deep investigation. In this regard, we have also took part to the theoretical and experimental studies on both active and passive plasma lenses to understand their effect on the beam quality and pave the way to their integration in conventional transport beam lines. For this reason different capillaries, in terms of size and material, have been investigated with different high voltage discharge circuits to ionize the hydrogen gas filling the capillary. The discharge phenomenon deserves deep investigation in particular for plasma-filled capillaries for plasma lenses, setting the initial conditions and therefore the uniformity of the plasma density, which in turn manifests itself in the linearity of the magnetic field. In addition, because of the nature of the gas-guiding structures used, detrimental effects on the beam stability due to wakefields might rise up requiring careful attention to minimize them.

Start-to-end simulation studies, together with an extensive experimental campaign, are typically performed to set the transfer line downstream from the plasma capillary to transport and match the plasma-accelerated witness beam into the undulator chain. We have successfully measured for the first time the exponential growth of the gain of SASE Free Electron Laser radiation at 820 nm. Results, compared to FEL simulations, have highlighted a very good agreement with measurements.

The obtained results indicate that the high-quality of the plasma accelerated beam (with low energy spread and emittance), accompanied by the high stability and reproducibility of the entire acceleration process, allowed to transport the beam along the undulators beamline and amplify FEL light in the near-infrared range. Considering the continuous efforts of the research community to develop next-generation ultra-compact accelerators, these results represent a fundamental milestone and will contribute for their ultimate implementation in multidisciplinary facilities for user-oriented applications.

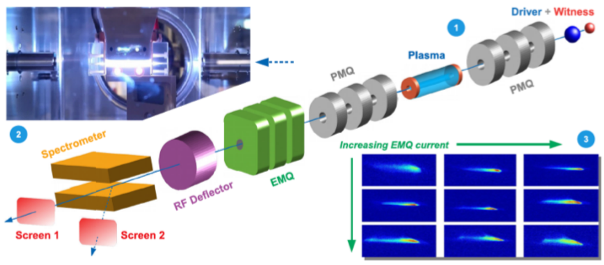

Figure 1: Plasma accelerator test bench at INFN SPARC_LAB. (1) The incoming driver and witness bunches are focused by permanent-magnet quadrupoles (PMQs) into the plasma accelerator module. A second triplet of PMQs is used to transport the bunches up to two diagnostics downstream (straight screen, screen 1) and bent (spectrometer screen, screen 2) beam lines. Electromagnetic quadrupoles (EMQs), a rf-deflector and a magnetic spectrometer allow to characterize the beam. (2) The plasma module consists of a 3 cm-long capillary where the plasma is produced by ionizing H_2 gas with a high-voltage discharge. (3) Typical quadrupole scan of the plasma accelerated witness performed on the spectrometer screen by varying the EMQ currents to reconstruct its normalized emittance.

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Accelerators for FLASH Radiotherapy

March 1, 2022

Radiation therapy (RT) is currently one of the principal techniques used for the treatment of cancer. The benefits associated with radiation therapy are widely recognized, but we have to take in account also the several risks, in the short and long term, associated with the treatment.

The FLASH therapy (FLASH-RT) is a promising cancer cure under development that spares healthy tissues from the damage of the ionization radiation maintaining the same efficiency of the conventional radiotherapy in the tumor cure. The FLASH irradiation delivers an almost instantaneous high radiation dose (> 1 Gy per pulse) in very short time (< 100 ms), producing a ultra-high dose rate (> 10^6 Gy/s).

In recent years, many studies about the radio-biological mechanisms underling the FLASH effect have been carried out from different research groups even if they remain mostly unknown. For this reason the investigation of new accelerators capable of producing FLASH doses are required.

In this scenario, at SBAI Department - Sapienza University we designed a novel linear accelerator (LINAC) dedicated to FLASH irradiation. It consists in a S-band (2.998 GHZ) standing wave bi-periodic structure working in $\pi/2$ mode [1,2] and developed in collaboration with SIT Sordina IORT Technologies SpA company. The LINAC was installed at Institut Curie in Orsay (France) in 2020.

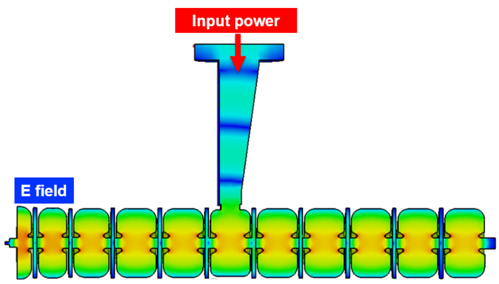

Figure 1: Electric field in the structure with accelerating and on-axis coupling cells.

The electromagnetic field inside the structure is excited by an RF waveguide (WR284 model), matched to the LINAC through a tapered section, that feeds the power into the cells. All cells are axially attached to each other and they are coupled mainly via magnetic fields through properly designed coupling holes located off-axis and secondarily via electric field through the cell's irises.

We performed different electromagnetic studies of the structure by using the code CST to optimize the main RF parameters (as summarised in Tab.1), and beam dynamics simulations with Parmela and E-gun to maximize the beam transport and energy.

Figure 2 shows the electric field on the LINAC axis after several iterations.

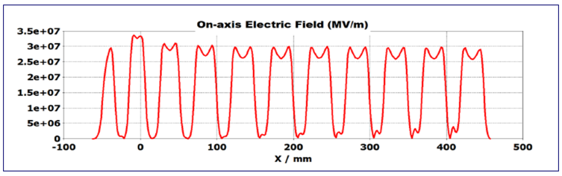

Figure 2: Electric field on the LINAC axis.

Frequency	3.001 GHz
Magnetron Power	3.1 MW
Number of Cells	11
Linac Length	67 cm
Output beam energy	7 MeV
Output beam current	> 100 mA
Electron beam capture	> 40%
Quality factor Q	14877
Shunt impedance r	77.5 $M\Omega/m$

Table 1: LINAC main parameters.

In order to minimize the overall dimensions and to obtain a compact structure, we performed an upgrade to C-band technology (5.712 GHz). Starting from the S-band (2.998 GHz) accelerator's structure we scaled down the geometric dimensions to get C-band design. Also in this case we have considered a standing wave, bi-periodic structure with $\pi/2$ mode of operation. The manufacture of a prototype of the LINAC at 12 MeV was carried out and low power RF test have been performed in Particle Accelerator Laboratory of SBAI department.

To allow the implementation of the FLASH Therapy concept into actual clinical use, it is necessary to have an accelerator able to treat deep tumors and the energy of the electrons should achieve the range of 50-250 MeV. More and different solution for a VHEE machine are under development and future studies are required.

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Neutral particles detection in Particle Therapy treatments

External Beam Radio Therapy is an effective way of controlling the tumor growth in combination or alternative with respect to other oncological treatments like surgery and chemotherapy. EBRT, so far, has reached a high technological readiness level and is exploited in many treatment centers with outstanding results. However there is still room for improvements, and two crucial areas in which urgent development is needed are the monitoring of proton therapy treatments and the detection of secondary neutrons producing during EBRT sessions.

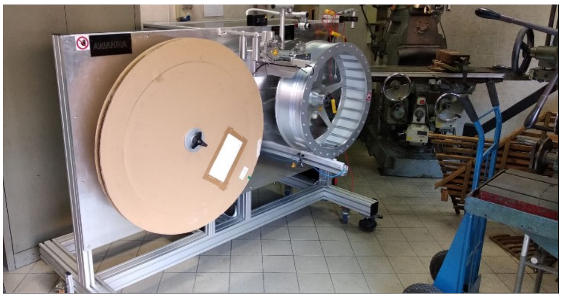

Figure 1: Wiring machine installed at the SBAI department.

The SBAI research group actively contributed to this latter field developing a neutron tracker that exploits the detection of two consecutive elastic scattering interactions of neutrons with matter to measure the neutron direction and energy. Neutrons pose in PT applications a serious problem both to the radioprotection optimisation and also to the secondary neoplasm insurgence due to the dose delivered far away from the target volume: neutrons are the only particles that can deliver significant doses far away from the target position and knowing their production point and energy spectrum would be crucial for particle therapy applications. The MONDO project [1,2] made a significant step ahead: the fiber winding machine needed to produce the full detector has been designed, produced, installed at SBAI and tested (see Figure 1) to build a prototype of the detector with small dimensions to be used for wiring testing purposes. The SBAM sensor (the readout chip that will be needed to acquire the signal produced by the recoil protons inside the fibres) has also been designed and a prototype has been tested.

At SBAI, also the first challenge has been addressed trying to exploit the prompt photons produced by the protons interaction with the patient tissues to monitor the beam delivery and the dose absorbed by the patient.

The SBAI research group contributed actively to an INFN project (call from CSN5) named PAPRICA (Pair production imaging chamber) in which the possibility to monitor proton treatments by means of detecting secondary prompt gammas was explored [3]. As such

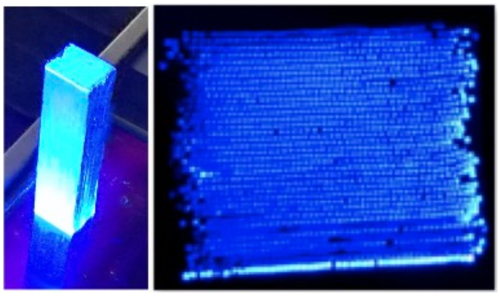

Figure 2: View of the first small prototype of a fiber detector to be used for secondary neutron production measurements.

photons have energies of few MeV a converter material of high Z was used to maximise the pair production probability and then an electron tracker made with the ALPIDE technology as well as an LSO calorimeter for electrons energy measurements were designed, produced and assembled at the LNF of INFN and at SBAI starting from 2019.

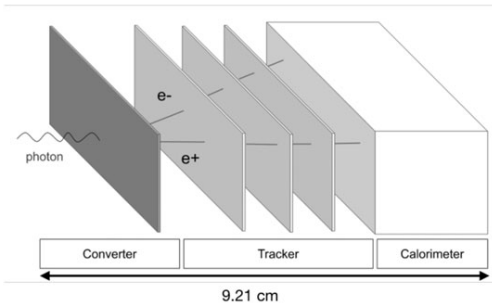

Figure 3: Scheme of the PAPRICA experiment detector. The incoming photon, the converter plane, the tracking planes and the calorimeter are shown.

A test beam is scheduled at the BTF - LNF facility in frascati to evaluate the detector electron tracking performance before a final test in a real PT evnironment using proton beam at the CNAO (Pavia) centre.

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Applied physics for the environment and particle accelerators

Our research activities are based on the use of the electromagnetic radiation as a diagnostic or as a driver to monitor or excite a particular system. We study with particular attention the potentiality of the use of Terahertz radiation. This radiation and therefore the technological development that follows is becoming more and more important nowadays because it finds applications in many research fields of basic and applied science e.g. spectroscopic characterization of given targets, imaging for medical and cultural heritage and in accelerator physics etc.. THz waves, (0.1-10)THz, offer innovative sensing technologies providing information unavailable through conventional analytical methods. THz radiation has a high level of discrimination in the rotational and vibrational transitions of bio-molecules and can therefore be used for identification and characterization. THz is sensitive to polar molecules such as water while interacting only weakly with non-polar molecules, such as plastic and ceramic, and is reflected by most metals. Therefore, THz spectroscopy has the big advantage in that it can be used for environmental monitoring through common packaging materials. In addition, THz is less affected by scattering than infrared and this makes it particularly suitable for the air-quality monitoring. THz waves are non-invasive since they are not responsible for light ionization and damage to biomolecules and can propagate through inflammable liquids without causing combustion.

Most of the studies we performed are dedicated to the applied physics for the environment e.g. monitoring of air pollutants pesticide and bio-hazard [1, 4] , for cultural heritage [2] and for accelerator physics [5, 7]. We also study different methods to produce and manipulate structured intense light pulses [3] that can be useful to investigate particular state of matter [4] and also for specific application as for example in the accelerator physics [6, 3].

Several other studies regarding the evolution of intense light pulses and their interaction with matter have been performed, e.g. [8, 9] but not presented in this text.

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http://sapienzaterahertz.sbai.uniroma1.it/

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Radiation protection

The research activity has three main objects: development and set-up of instrumental devices concerning radon issues, development and set-up of devices for Special Nuclear Materials safety and security, and design of a new facility for radiopharmaceuticals production by neutron activation with TRIGA nuclear reactor at ENEA Casaccia.

As radon issues are concerned, in the last three years research projects were carried out in collaboration with CNR (the Italian National Research Council) and ISS (the Italian National Institute of Health). One of the most important project was the design, realization and commissioning of a radon calibration chamber to test radon detectors, Figure 1.

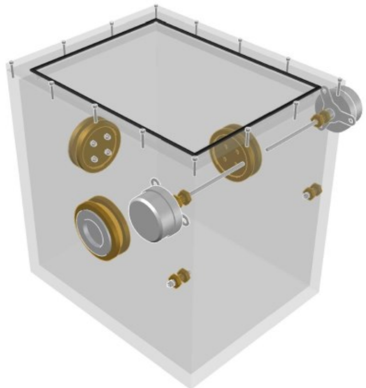

Figure 1. The radon chamber.

The main innovation is the way radon activity concentration is regulated inside controlled atmosphere. The system allows to establish a wide range of concentration trends. Such result is obtained by means of a single radium source placed outside the control volume, and the contemporary operation of two air-flow circuits, the first one connecting the source to the chamber, the second one connecting the chamber to the outdoor. The detector can be used for fast and quantitative analysis to estimate radon equivalent concentration, or to determine the effective dose associated to measured potential alpha energy concentration. As a remedial action against radon issues, an electrostatic precipitation system for reducing effective dose due to radon progeny in air was designed and realised. It is a single-stage and multi-duct, parallelepiped electrostatic precipitator (ESP). The results obtained during the experimental campaign revealed a net reduction of the effective dose intake due to the ESP radon daughters' sequestration, reaching up to ~38%.

As regards Special Nuclear Materials security, the design of the Neutron Active Interrogation system (NAI), was carried out in the frame of EC Research Project "EDEN" (https://eden-security-fp7.eu). NAI has been conceived and optimized to identify transuranic-based Radioactive Dispersal Devices potentially hidden in packages. Fissile material detection is made using the Differential Die-Away time Analysis (DDAA), an active neutron technique based on the difference among the die-away times of fast interrogation neutrons and prompt fission neutrons induced by thermal neutrons in the moderating system.

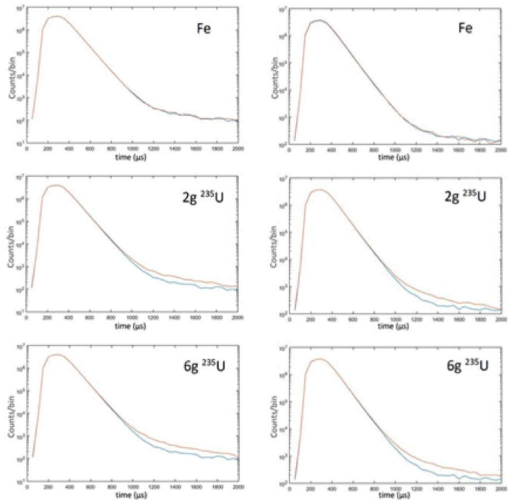

Figure 2. Differential Die-Away time Analysis curves for three different samples.

As regards Radiopharmaceutical production, a feasibility study concerning tecnetium-99m production by neutron activation has been carried out in collaboration with ENEA, in the framework of the research contract SBAI – ENEA (2019). For reducing the issues due to lower specific of neutron activation vs. nuclear fuel reprocessing a new type of "gel" 99Mo – 99mTc has been developed.

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Authors

R. Remetti

A Treatment Planning System for Intra Operative electrons Radio Therapy applications

Advanced radiotherapy techniques use complex beam delivery systems in order to obtain high tumor control probability with reduced normal tissue complication rate. The software (Treatment Planning System, TPS) that provides to the accelerator control system the position, intensity and direction of the beams to be delivered is crucial to achieve the patient therapeutic need. Regardless which kind of radiotherapy is considered the TPS computation is based on the imaging of the patient and on the characteristics of the beam delivery system. The main TPS component is the kernel of the compute the dose released by the beams in the patient. In clinical practice analytic algorithms are used to reproduce the dose deposition, approximating the patient tissue with water. In a limited number of complex cases, Monte Carlo (MC) simulations are instead used. These very accurate tools are not routinely used in clinical practice, due to the large computational resources needed to simulate a whole treatment plan. At the moment, one of the main TPS improvement is the computing time reduction keeping as higher accuracy as possible.

In this framework, the code FRED (Fast paRticle thErapy Dose evaluator)[1,2] has been developed at SBAI to allow for a fast optimization of treatment plans while profiting from the dose release accuracy of a Monte Carlo (MC) tool. Within FRED, the proton, carbon ions, photons and electrons interactions are described with the precision level available in leading edge MC tools used for medical physics applications, with the advantage of reducing the simulation time up to a factor 1000. In this way it allows a plan MC recalculation in a few minutes on GPU (Graphics Processing Unit) cards, instead of several of hours on CPU (Central Processing Unit) hardware.

The use of this MC-on-GPU based software is opening new opportunities also in the planning of Intra Operative Radio Therapy (IORT)[3], especially in the context of IORT-Flash Therapy[4] applications.
The IORT is a technique that involves precise delivery of a large dose of ionizing radiation (4-12 MeV electrons beam) to the tumour or tumour bed during surgery in order to eradicate the microscopic residual tumor cells left after surgery. Currently the two main IORT limitations are the unavailability of a TPS and of a report of the dose delivered, needed by law from 2020 (European 2013/59/EURATOM Italian D.Lgs 101/2020). Such limitations are both due to the very limited amount of time available (order of 1 minute) during the surgery to obtain both the imaging of the surgical field and the TPS computation.

At SBAI, in close collaboration with the S.I.T. company, a TPS that makes use of an on-line, 'in-site' ecographic imaging input is being developed. Exploiting the FRED-em implementation and the GPU hardware, the dose volume histograms (DVH) needed to plan a treatment can be obtained in a matter of seconds allowing to explore different beam energies and delivery positions that can optimise the PTV coverange and OARs sparing. The preliminary results obtained using an ecographic-like input of a breast cancer treatment are shown in Figure 1. The figure shows the dose distribution obtained using electrons of 8 MeV energy and an applicator of 7 cm radius. Similar distributions can be obtained for different energies and geometrical conditions allowing to optimise the treatment within the required time.

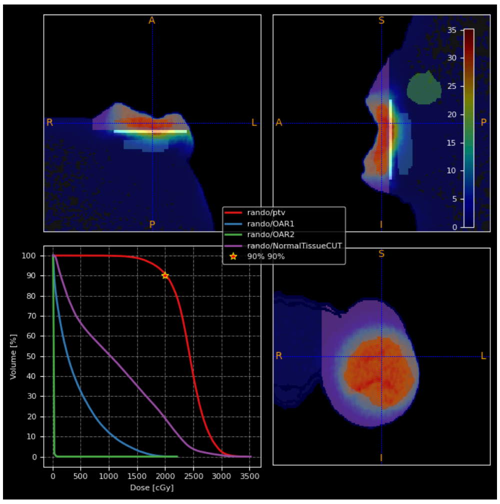

Figure 1: Example of breast cancer treatment. The dose distributions for 8 MeV electrons are shown in three different views, as well as the related DVHs used for the treatment optimisation.

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Monte Carlo particle transport on GPU for particle therapy applications.

Particle therapy is using beams of accelerated charged particles to reach deep seated tumors inside the human body. This approach can be as effective in controlling the tumor as conventional radiotherapy using gamma rays. The main advantages are the high conformity of the dose distribution to the planned target volume, and a better preservation of healty tissues. To achieve these goals, accurate planning and delivery of the treatment plan are mandatory. The planning and verfication of a treatment are bestly done using Monte Carlo (MC) simulation of particle matter interaction. This is a very accurate modelling of particle trasport, taking into account the fundamental processes that lead to particle energy deposition and trajectory deflection inside the human body. Also nuclear interactions are relavant in the therapeutic energy range used for particle therapy (typically a few 100 MeV for nucleon). Nuclear elastic and inelastic interaction are leading to primary beam conversion into a secondary radiation field, whose physical and biological interaction with the human cells determines the actual effectiveness of the treatment in damaging and controlling the cancerous cells.
Monte Carlo simulations are rather long, since many particles (order of a few 100 million per treatment) have to be tracked in order to reduce the statistical fluctuations. On standard CPU hardware we can expect the *de facto* standard codes to track about 1000 particles per second. Hence a significant number of computing cores are needed to reduce the computation time to the typical timeframe needed for clinical applications, namely a fraction of a hour.

At SBAI Department - Sapienza University we developed the FRED code, which is a new MC simulation platform for treatment planning in ion beam therapy. The code can transport particles through a 3D voxel grid using a class II MC algorithm. The tracing kernel can run on GPU hardware, achieving 10 million primary/s on a single card. This performance allows to recalculate a proton treatment plan at 1% of total particles in just a few minutes.
Following the first publication of the model in 2017, we continued the developement of the code to further improve accuracy and tracking performance at the same time. In order to allow simulation of primary Carbon ion beams, the stopping power and energy loss fluctuations were implemented and validated against standard MC codes for all stable light ions and their isotopes with atomic number $Z \leq 6$. Also the Multiple Coulomb Scattering algorithm was implemented and verified for light ions, using a single central Gaussian approximation of the angle distribution with a scaling factor the was tuned against standard MC codes [1].
The nuclear elastic module was also revisted and improved to describe the scattering of protons off any given nucleus. The angle distribution of the scattering angle (Fig.1) was modelled using the parametrization proposed by J. Ranft, and it was finely tuned against ICRU tabulated cross-sections. The kinematics of the nuclear event was solved in the center of mass frame, and then Lorentz transformed back to the laboratory frame [2].
Collaboration with the oncological treatment centres of CBB (Poland) and MAASTRO (The Netherlands) led to the implementation and validation of FRED into the clinical quality assurance workflow as an alternative dose engine with respect to the commercial tool used for planning [3].
The FRED code was also used to simulate a proton radiography setup in order to investigate the possibility to define a patient-specific HU calibration curve with the intent of improving the accuracy of proton beam range predictions, which is ultimately depending on the HU to tissue properties conversion [4].

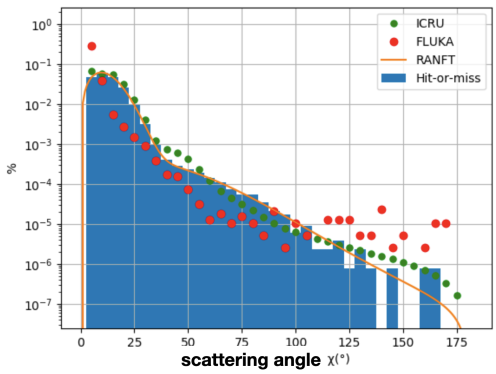

Figure 1: Proton nuclear elastic scattering: angle sampling.

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http://fred-mc.org

Particle Therapy treatments monitoring

Charged Particle Therapy (PT) is a technique for cancer treatment that exploits hadron beams, mostly protons and carbon ions and their energy loss in matter to achieve a high Tumor Control Probability while minimising the Normal Tissue Complication Probability. The highly localised dose release of primary beam particles and their large Relative Biological Effectiveness can be used for the treatment of radio-resistant tumors and tumors that are located nearby Organs at Risk (OARs). However the ballistic precision achievable with such projectiles calls for an unprecedented precision and control on the volume that is effectively targeted during the treatment. As the beam is stopped within the patient tissues, the monitoring of the treatment has to be performed exploiting the secondary radiation produced by the beam interactions with the crossed tissues.

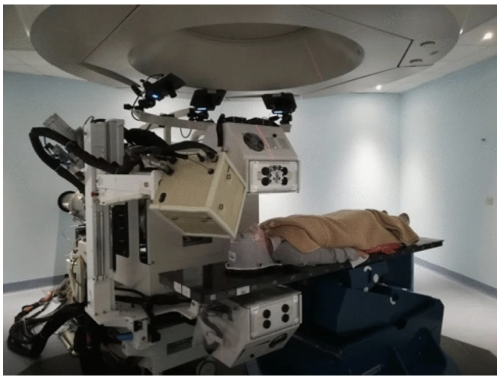

Figure 1: View of the INSIDE cart with the DP (beige box) installed in the CNAO treatment room n.1. The image shows a view of the first patient treated with ^{12}C ions.

The authors of this contribution have a long standing experience in the field and addressed in the last years different challenges posed by the PT treatments monitoring [2,3]. In particular, the dhe Dose Profiler project [1,4,5] aimed at monitoring the inter-fractional changes occurring in the patient morphology when undergoing Cabon Ion treatments at the CNAO centre. The DP was part of a larger project (INSIDE) aiming to monitor also proton treatments using PET photons and underwent a clinical trial starting in 2019. The DP exploits charged particles (mostly protons) produced by the beam interaction with the patient tissues to monitor the beam path inside the tissues, allowing to monitor changes occurring during the treatment delivery that can last up to 4 weeks. The detector, built at SBAI in 2017, was finally shipped to CNAO and used to monitor patients starting from 2019. Figure 1 shows the first patient treated at the CNAO centre with carbon ions in end of July 2019, that was monitored by means of the DoseProfiler [1].

Ten patients, enrolled in a clinical trial, were monitored using the dose profiler in order to quantify the potential of the charged particles monitoring technique in identifying the insurgence of morphological changes during the treatment that could alter the plan with respect to what was planned on the basis of the first image acquired at the planning stage. Figure 2 shows, for the fourth monitored patient, the modulation of the secondary particles production point as a function of time that identifies a clear change in the patien morphoilogy that was correlated to a change in the frontal sinuses of the patient, as documented and detailed in [1], proving the technique potential.

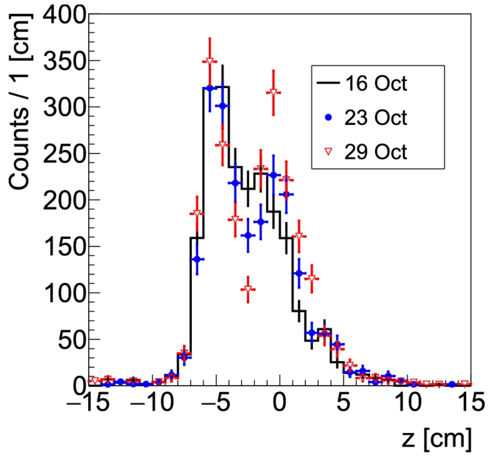

Figure 2: View of the INSIDE cart with the DP (beige box) installed in the CNAO treatment room n.1. The image shows a view of the first patient treated with ^{12}C ions.

The results have been published on nature scientific reports [1] and the second half of the clinical trial (that was scheduled in 2019 and was stopped due to the covid-19 pandemic) is about to start.

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Quantum Engineering

Implementing "Quantum Science" into innovative products capable of stimulating growth and creating new jobs is undoubtedly a major challenge, which can only be won if the link between the industrial production part and the scientific part is strengthened. In this context, in recent years a synergy has developed between SBAI - Nonlinear Optics Laboratory (C. Sibilia) and Quantum Technologies Lab - Electronics Division - LEONARDO (F.A. Bovino). The Quantum Technologies Lab - Electronics Division of LEONARDO, holds a leadership position in the national/international field, conducting advanced research in the fields of Quantum Information and Communication Technology, which led to the creation of the only two Italian products in the field of Quantum Cryptography, the most recent of which is the Q-KeyMaker®. The two devices were developed as part of the projects funded by the Ministry of Defense (MD), namely: "QUCRYPT-D (" Advanced Quantum Cryptography ") and" QUCRYPT-NET.

MD's interest in Quantum Technologies and for research applied to security has given rise to the funding to SBAI of numerous programs that have allowed the cementing of cooperation with the Quantum Technologies Lab-Electronics Division-Leonardo, such as the SORGENTI project ("Optical sources for safety"), the MARINE project ("Materials with negative refractive index"), the important COPERNICO project ("Chip for advanced quantum computation and sensors in the near-medium IR") and more recently the “QUASAR” project (Quantum Safe Network ”) which sees the collaboration with the Scuola Superiore Sant'Anna of Pisa, the CNIT (Consortium for Telecommunications), the University of L'Aquila and the University of Naples Federico II.

Quantum computing has attracted a lot of interest in the last 15 years, mainly due to its ability to factor large numbers in polynomial times and its efficiency in simulating the dynamics of complex quantum systems. In this regard, circuits have been designed and built that exploit light for the coding of quantum information, based on a patent by F.A. Bovino-Leonardo Company (EP3109803 - STRUCTURE AND METHOD FOR PROCESSING QUANTUM INFORMATION). It is a revolutionary computing architecture that allows the so-called IntraSystem Entanglement to be created. Entanglement represents a key element for quantum information processing and in this new architecture the correlation properties are not related to the internal degrees of freedom of the particles, but are "inprinted" on an optical circuit. Thanks to this idea, “universal quantum logic gates”, complex circuits such as the Quantum Entangler shown in the figure 1, and Quantum Teleportation systems have been created. The race for the development of quantum computers is underway: NASA and GOOGLE already use the quantum computer of the D-WAVE costing 10 million dollars, bulky and operating at temperatures close to absolute zero. Our goal, retracing the example of Olivetti's 101 Program, is to create the QUANTIUM, the first quantum PC.

Quantum Engineering also involves the development of highly sensitive optical sensors with the development of innovative magnetic devices and the study of new materials.

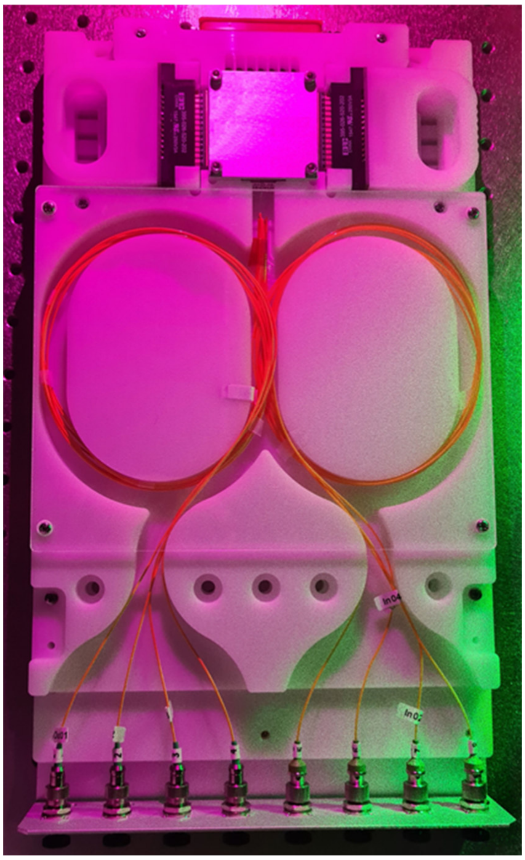

Figure 1. Entangled Plug & Play State Source for Device Independent Quantum Cryptography, developed in the Quantum Photonics Lab of the SBAI - SAPIENZA Department, as part of the "QUASAR" project.

Authors

C. Sibilia, F. A. Bovino

The FOOT (FragmentatiOn Of Target) experiment

Charged Particle Therapy (PT) uses proton or ^{12}C beams to treat deep-seated solid tumors, and due to the advantageous characteristics of charged particles energy deposition in matter, the maximum of the dose is released to the tumor at the end of the beam range, in the Bragg peak region. However, the nuclear interactions of the beam nuclei with the patient tissues induce fragmentation both of projectile and target nuclei and need to be carefully taken into account when planning the treatment. In proton treatments, the target fragmentation can induce low energy, short range fragments along all the beam path, that may deposit a non-negligible dose in the entry channel. On the other hand in treatments with ^{12}C, or other possible ions of interest, like ^{4}He or ^{16}O, the main concern is long range fragments, produced by projectile fragmentation, that release their dose in the healthy tissues beyond the Bragg peak. The same nuclear process is of increasing interest for radiation protection in human space flight, in view of deep space missions. In particular ^{4}He and high-energy (E) and charge (Z) particles (HZE), mainly ^{12}C, ^{16}O, ^{28}Si and ^{56}Fe, provide the main contribution to the equivalent dose in deep space. The study of the impact of these processes, of interest to both PT and space radioprotection, at present suffers from the still significant lack of experimental data concerning the relevant nuclear cross sections, while the available computational models are not yet sufficiently reliable. The FOOT (FragmentatiOn Of Target) experiment, approved and funded by INFN in 2017, aim to study these nuclear processes and measure the corresponding fragmentation cross sections with a goal of 5% on the maximum uncertainty , needed to match the required 3% precision on the delivered dose in a Radio-Therapy treatment planning [1]. The FOOT detector, shown in Figure 1, consists of an "upstream region" composed by the pre-target detectors, aim to monitor the impinging beam, and, downstream of the target, a setup based on a magnetic spectrometer, coupled with detectors for tracking and detectors optimized for the identification of fragments. A research effort has been devoted, within SBAI, to the experimental apparatus design, to several data taking campaigns for the test and the calibration of the detectors [2], [3] and to the development of reconstruction algorithms for the identification of the fragments in the FOOT setup. Fragmentation cross section measurements with a preliminary FOOT setup have been published [4].

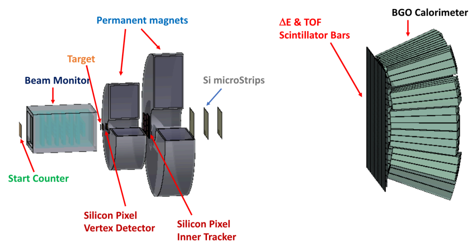

Figure 1: FOOT final detector

The FOOT detector is a "movable" apparatus designed to fit the space limitations set by the possible experimental rooms where ion beams of therapeutic energies are available. In particular CNAO (Pavia, Italy) experimental room is well suited for the FOOT physics and purposes. On the other hand the detector technologies and readout systems chosen to reach the required performances, in particular in terms of Time-Of-Flight and momentum resolution, limits the FOOT rate capability to some kHz. The request of working at low rates asked for the development in CNAO experimental room of a beam monitor working in this regime. The standard beam monitors used in the treatment rooms of CNAO are ionization chambers fully efficient only for rates greater then about 10 MHz. For this reason the SBAI research team, with the technical support of Marco Magi, developed a monitor based on two X-Y views of plastic scintillating fibers exploiting SiPMs as photon detectors and a read-out system of ASICs and FPGA. The final detector will be installed in CNAO experimental room at the end of 2022. The direct SBAI researchers contribution in the three years 2018-2020 is related to the following items: the experiment and collaboration coordination (V. Patera as collaboration spokesman), the Start Counter construction and operation (A. Sciubba) as well as the interaction region construction and detector integration, the reconstruction software coordination and develpment (A. Sarti), and the development of the low intensity beam monitor for CNAO experimental room (M. Toppi).

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Multiscale Non Equilibrium Green Function Approach for Protein Sequencing in Graphene Nano-Ribbons Devices.

The knowledge of the protein primary structure is crucial to identify the post-translational modifications or mutations affecting the proteins 3D structure and their behavior. However current protein sequencing methods represent serious drawbacks for practical application of proteomics in medicine and new sequencing methods are needed to support this challenge. Measuring the transversal tunneling current across two nano-electrodes during the protein translocation can succeed because the signal depends on the chemical and physical nature of the amino acids (AAs) in the nanogap. The usage of 2D graphene nano-ribbon electrodes allows the atomistic resolution (Fig. 1). A multiscale approach is adopted using classical Steered Molecular Dynamics to perform the translocation and the Non Equilibrium Green Function (NEGF) method at the Density Functional Theory (DFT) level for the tunneling current. The DFT-NEGF transmission function is

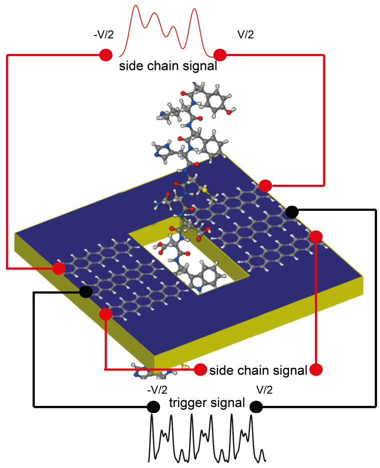

Figure 1: Ideal graphene nanoribbons nano-gap device for protein sequencing

$$T(\varepsilon) = \mathrm{Tr}\left[G(\varepsilon)\Gamma_L(\varepsilon)G^{\dagger}(\varepsilon)\Gamma_R(\varepsilon)\right] \quad (1)$$

where $G(\varepsilon) = \lim_{\eta\to 0^+}(\varepsilon + i\eta - H)^{-1}$ is the Green's function of the device and $\Gamma_{L(R)}(\varepsilon) = i[\Sigma_{L(R)}(\varepsilon) - \Sigma^{\dagger}_{L(R)}(\varepsilon)]$ is the left(right) coupling function. They are obtaned at the DFT level. Then the tunneling current is calculate through the Landauer-Büttiker formula for an external bias voltage V:

$$I(V) = \frac{2e}{h}\int_{-\infty}^{+\infty} d\varepsilon T(\varepsilon, V)\left[f(\varepsilon-\mu_L) - f(\varepsilon-\mu_R)\right] \quad (2)$$

where $f(\varepsilon)$ is the Fermi-Dirac distribution function and $\mu_{L(R)}$ is the electrochemical potential of the left(right) electrode. The tunneling signal from the peptide backbone is an atomistic resolved periodic signal with well defined maxima related to the peptide bond features of different model peptides with small AAs, either neutral (glycine and alanine) or polar (asparagine, aspartic acid and serine) (see Figs. 2, 3). Moreover it is not affected by the polar nature of the AAs side chain.

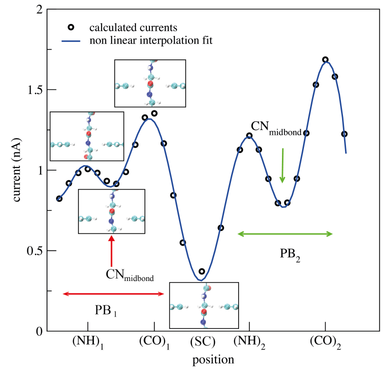

Figure 2: Tunneling current from a Gly homo-peptide

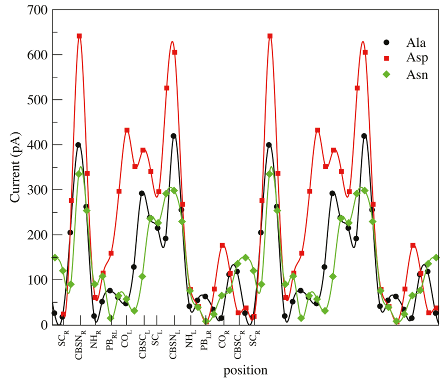

Figure 3: Tunneling current from Ala, Asn and Asp homo-peptides

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Laboratories and facilities

Laboratory for non-destructive analyses and archaeometry – Landa ”Sebastiano Sciuti”

The laboratory has a long-lasting experience in the field of the archaeometric study of Cultural Heritages. By using non-destructive analytical methods mural and easel paintings, ceramics, metal and stone artifacts, manuscripts books, etc. are analyzed in order to obtain information on the materials constituting the artifacts and on the techniques employed to realize them.
The laboratory takes part of the Research Infrastructure of the Center of Excellence DTC Lazio (network R6 - Chemical and physical sciences and technologies).
Equipment: All the equipment available in the laboratory is portable and allows to perform the analyses in situ.
Energy dispersive X-ray fluorescence spectroscopy (ED-XRF)
It allows to obtain information on the chemical elements present in the analyzed material and, in some cases, on their concentrations. The spectrometer is constituted by a miniaturized X-ray generator and a silicon drift detector integrated with a multichannel analyzer. It allows the detection of all the elements starting from aluminum with a limit of detection ranging from 10^2 ppm to 10^3 ppm.

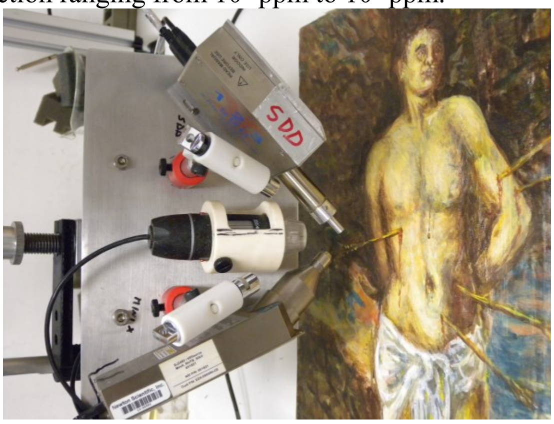


Figure 1. Energy dispersive X-ray fluorescence spectrometer

UV-Vis-Near Infrared (NIR) Multispectral Imaging system
The system is devoted to the in situ analysis of easel and mural paintings, manuscripts and books. It is equipped with a Peltier cooled CCD camera, halogen lamps, UV and Vis LED's and a set of 20 narrow interferential filters from UV to NIR. It allows to acquire reflectance or UV induced fluorescence images corresponding to narrow portions of the spectral region and from those to obtain information on the organic and inorganic materials that constitute the pictorial layers or to reveal preparatory drawings and "pentimenti".
UV-Vis-NIR spectrophotometer
For reflectance and absorbance measurements and spectrofluorimetry.
Raman spectrometer
Portable Raman spectrometer equipped with a laser at 532 nm. It is used for the identification of chemical compounds.
Digital microscope
Dinolite AM7915MZT-Edge, magnification: 10-200X. It allows to acquire macrophotographs in situ.
Collaborations:

- Avignon University
- University of Rome "Tor Vergata"
- LNF, INFN
- Accademia Nazionale di San Luca

https://www.sbai.uniroma1.it/strutture/laboratory-non-destructive-analyses-and-archaeometry-landa

LEOS*MS (Laboratory of Electrochemistry, Organic Synthesis & Mass Spectrometry)

LEOS*MS Facilities

- Spinsolve 60 benchtop NMR spectrometer
- Perkin Elmer 841 InfraRed Spectrometer
- Perkin Elmer Series 2 HPLC Liquid Chromatograph apparatus
- AMEL System 5000 Multifunctional Electrochemical System
- AMEL 2551 potentiostat/galvanostat apparatus
- AMEL 552 potentiostat equipped with Amel 566 function generator and Amel 563 multipurpose unit
- AMEL 472 coupled with a digital x/y recorder AMEL 863 for potentiodynamic methods (Voltammetry) performed by a three-electrode multipolarograph
- AMEL 552 potentiostat coupled with an integrator AMEL 731 and an x/y recorder LINSEIS L250E for CPE (controlled potential electrolyses) for spectroelectrochemistry in UV-vis modified cell
- Electrodes and microelectrodes for Voltammetric Techniques and Electrolysis (RVC, GC, Au, Pt, Mg, ITO)
- GC-MS Hewlett-Packard 5890 series II Gas Chromatograph coupled with a Hewlett-Packard 5871 series II quadrupole Mass selective detector
- HPLC 1525µ Waters chromatographic separation module, coupled with a photodiode array detector 996 PDA Waters and a Quattro Micro Tandem MS/MS detector with an ESI source (Micromass, Manchester UK)
- GC-MS System Clarus 500 MS Turbo (PerkinElmer Instruments LLC, U.S.A.)
- Agilent 8453 diode array spectrophotometer.
- Ultrasound high-energy sonicator
- Ultrasound bath apparatus
- Complete experimental setup for chromatographic techniques (TLC, Flash)
- Complete experimental setup for synthetic organic chemistry
- Melting point apparatus SMP2 (Stuart Sci.)
- ALC Centrifugette 4206
- ALC Centrifuge 4222 MKII
- Freeze Dryer system
- Schlenk apparatus for the manipulation of air-sensitive compounds (vacuum or inert gas atmosphere)

LEOS*MS Expertise

The group has thirty years of experience in the field of organic electrochemistry, particularly for the synthesis of materials for organic electronics, small molecules of industrial and pharmaceutical interest, incorporation of carbon dioxide in organic compounds. The research group has specific skills in organic synthesis, electrochemical characterization of organic molecules and salts, also in view of their application in organic electronics. The group has always carried out training of young researchers in the field of organic and electro organic synthesis.

Aims of the **LEOS*MS** are: Chemical syntheses, characterization and electrochemical studies of new organic compounds and nanocomposite materials used in photovoltaics, OLEDs, plastic scintillators, erbium infrared emitters, photodetectors, semiconductors for sensor applications, and more. To study organic and redox reactions by electrochemical techniques, in particular to carry out the electrochemical synthesis of fine chemicals and of products of interest for pharmaceutical and chemical industry. Development of electrochemical syntheses in ionic liquids as greener solvents than VOCs. HPLC-PDA-MS/MS analysis provides information on the chemical composition of different matrices of interest, as the products mixture resulting from organic reactions, or real matrices from food and beverages industry, paying particular attention to the antioxidant phenolic components for nutritional and waste recovery purposes, to name a few.

Molecular Photonics Laboratory

The Molecular Photonics Laboratory (MPL) gathers equipment, expertise and experiments used for the study of the linear, nonlinear, photoluminescence and electroluminescence properties of molecular and polymeric organic materials. Such materials are used for the fabrication of integrated optical devices, organic light emitting diodes (OLED) and dye-sensitized organic solar cells (DSSC).The laboratory expertise has been developed since 1992, also in the frame of master of science and doctorate projects carried out in particular by students of the Electronic Engineering, Nanotechnology Engineering and Physics Courses.

Since 2007 the laboratory started migrating towards the field of Biophotonics, in which the materials are still organic but of biological origin. We worked hard to pursuit such a transition, which involved a modification of the experimental techniques and their integration with new expertise in chemistry and biochemistry. We believe the transition is now complete as witnessed by our latest publications in the field.

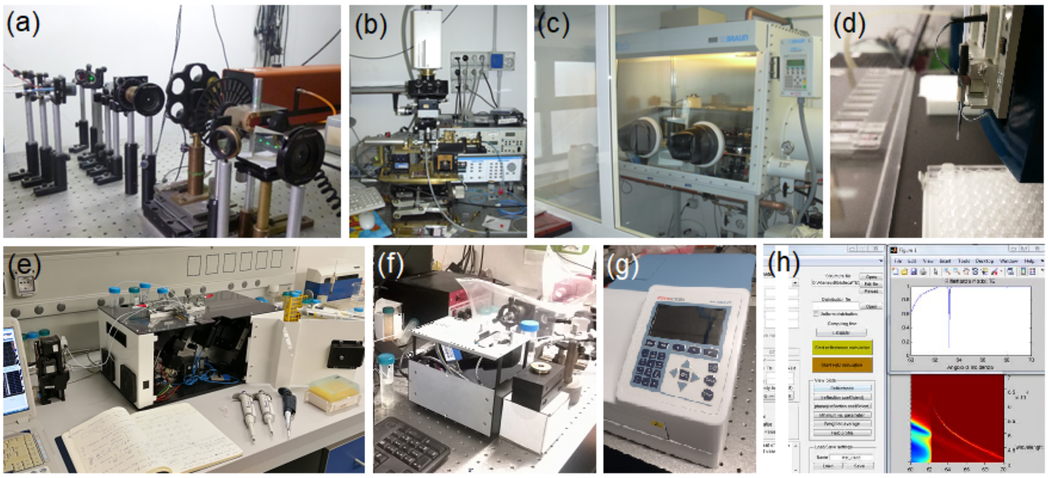


Figure 1: (a) Custom benchtop optical setups, (b) Integrated photonics setup, (c) Glove-box, with DC sputtering and spin coating systems, (d) Nano-bio-spotter, (e) BSW early cancer biomarker detection platform developed in the project BILOBA, (f) Infrared Surface Plasmon Resonance platform, (g) ELISA platform, (h) Custom and commercial tools for advanced numerical simulations in optics and photonics.

The MPL is equipped with the following technical instrumentation:

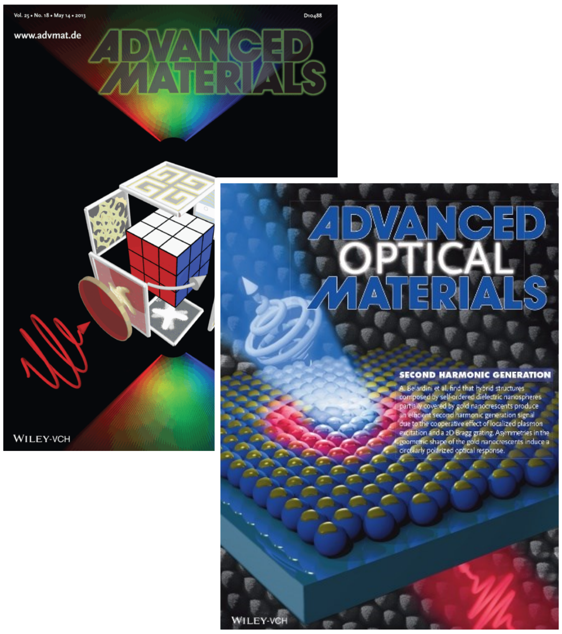
- CW He-Ne lasers (632.8 and 543 nm) and laser diodes (635, 670, 1300, 1550nm, tunable 1490-1590nm);
- optical components (mirrors, lenses, beamsplitters, polarizers, phase retarders, fibers, objectives) and mountings (manual/motorized) used to assemble benchtop laboratory setups in optics and photonics;
- complete experimental setup for the characterization of photonic integrated circuits, with microscope;
- equipment for the chemical functionalization of optical biosensors (gold/dielectric surfaces), with a glove-box;
- equipment for microfluidics (cells, motorized pumps, tubings, switches, valves, temperature control);
- GESIM nano-bio-spotter used to deposit antibodies, proteins and ss-DNA with high spatial resolution;
- Thermo-Fisher ELISA plate reader;
- Custom surface plasmon polariton and photonic crystal biosensing platforms;
- CW sputtering (gold) and spin coating systems;
- Range of didactic kits used in the optics and photonics courses, including a WEB accessible ellipsometer.

https://www.sbai.uniroma1.it/strutture/molecular-photonics-laboratory

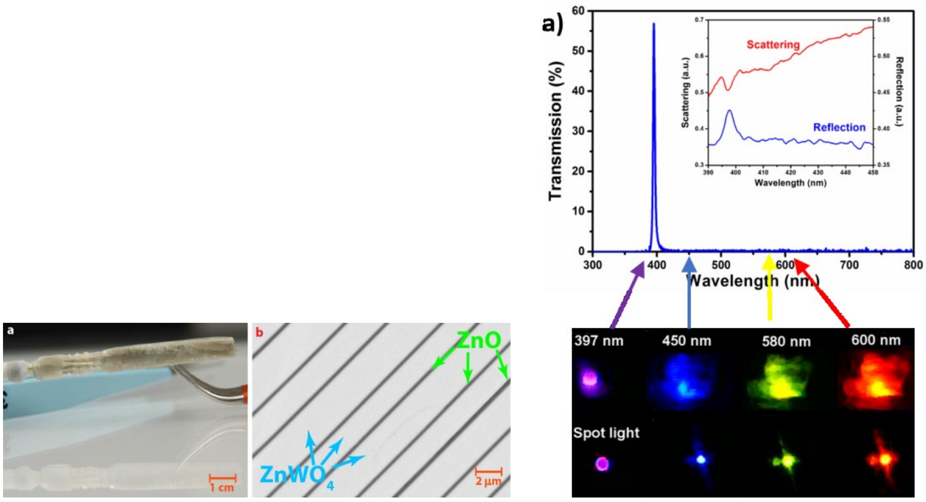
Nonlinear Photonics & Quantum Photonic Lab

The Nonlinear Photonics has been active for years in experimental research and in the modeling and simulation of nonlinear optical and optical processes and devices, with applications in nanophotonics, plasmonics and quantum photonics as:

- study and design of novel single photon emitters, nonlinear sources based on photonic crystals;
- Linear and Nonlinear optical filters for the manipulation of the electromagnetic radiation in different spectral ranges.
- The laboratory is equipped with numerous computers running both commercial (Optiwave, Comsol Multiphysics, Lumerical), as well as customized software.



Simulations and Experiments on nonlinear “artificial “chiral materials

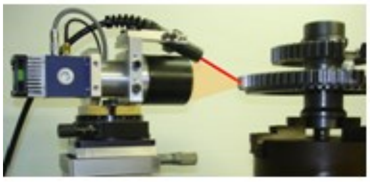
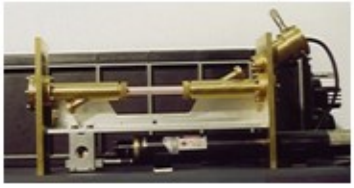
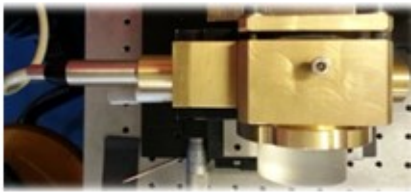


Filtering properties of lamellas of ZnO/ZnWO4

(with Center of Excellence on Nanophotonics- ENSAMBLE3)

Photoacoustic & Photothermal Techniques for Nondestructive testing of materials

Web site: https //www sbai uniroma1 it/strutture/tecniche_fototermiche_fotoacustiche

In the PA&PT Lab the following techniques have been designed, realised, and optimized: UV VIS NIR photothermal deflection and photoacoustic spectroscopy, photothermal radiometry and infrared thermography, and standard optical techniques. Theoretical modeling and simulation tools for optical and thermal meta-nanomaterials are available in a protected area of the Lab.

Main applications in the PA&PT Lab: measurements of thermal diffusivity of materials; optical and infrared refectance, transmittance and absorbance; infrared signature of filters and targets; optical, thermal and hardness depth profiling in graded materials; detection of subsurface layers; analysis of traces of gaseous pollutants, optimization of photovoltaic cells, detection of dichroism and resonances in nanostructures, UV VIS NIR spectroscopy for agrifood, thermophysical properties of materials for nanophotonics and nanophononics.

Instrumental. Sources: Argon Ion Laser, INNOVA 70-3, CO2 CW Laser MPB Technologies 10W @10600nm, Laser diode, Coherent 2W @810nm, Laser diode, Hitachi 3mW @635nm, Laser diode, LaserMax Crisel 5mW@1310nm, He-Ne Meles Criot 5mW @633nm , Xenon Lamp.
Optics: Lenses, Interferential filters, mirrors, beam splitters, Monochromator (Jobin Yvon).
Detectors: Si and GaAs photodiodes. Pyroelectric sensor. HgCdZnTe IR detectors. Position sensors. Photomultiplier. Infrared Camera 8-14 μm.
Electronics: 2 Lock-in amplifiers. Digital oscilloscope Tektronix- - Microvoltmeter HP
Mechanics: 2 optical tables (Newport). Automatized rotation and translational stages.
Informatics: 4 PC desk-top. Software LabView.

Several research lines have been activated in the PA&PT Lab in order to carry on most of the activities done in the framework of the following national and international research projects:

a) 2010 - 2015. Research project funded by the Italian Ministry of Defense program PNMR 2008.55 "*FISEDA: Infrared selective filters for the reduction of the IR signature of targets*": Project leader C. Sibilia, Scientific Responsible R. Li Voti
b) From 2017. Research project funded by the Italian Ministry of Defense program PNMR 2014.061 "*SCHERMA: study of nanostructured and composited materials for thermal and electromagnetic shielding for the reduction of the IR signature*": Project leader C. Sibilia, Scientific Responsible R. Li Voti
c) From July 2017. Contract with BIFRANGI S.p.A. "*Radiometric apparatus for the nondestructive measurements of the hardness depth profiling for induction hardened steels components*": P.I. R. Li Voti
d) From April 2014 to March 2015 – Research contract with ITALDATA S.p.A. in the framework of the Co-Research funded by Filas S.p.A entitled: "*D.O.M. – Digital Object for Mobile learning*": P.I. R. Li Voti
e) From 2017. European project Ensamble "*Centre of Excellence for nanophotonics, advanced materials and novel crystal growth-based technologies*" funded Grant Number 763798 and leaded by C.Sibilia
f) From 2015. "*Framework Agreement on Strategic Cooperation*" between the Nanjing Institute for Product Quality Inspection and the Dipartimento S.B.A.I. in the field of NDT on products leaded by R. Li Voti.

Physics of semiconductors and nano-structures

The laboratory is mainly devoted to the study of the structural and the electronic properties of semiconductors and nano-sized materials, both from the experimental and the theoretical/computational point of view. Concerning the theoretical and computational physics activity, the laboratory owns a computational infrastructure with a total of more than 250 cores. A small high performing computing (HPC) cluster has been build in-house with four nodes (176 cores) with high speed infiniband interconnection and switch(see Fig.**??**(a)). The laboratory owns the equipment for structural analysis of materials and nano-structures through Transmission Electron Microscopy (TEM) (160 KV) [Fig. **??**(b) for], optical microscopy and Reflection High Energy Electron Diffraction (RHEED) [**??**(c)]. The laboratory owns the entire equipment needed to build and prepare samples for TEM, including the final ion milling stage [Fig. **??**(d)].

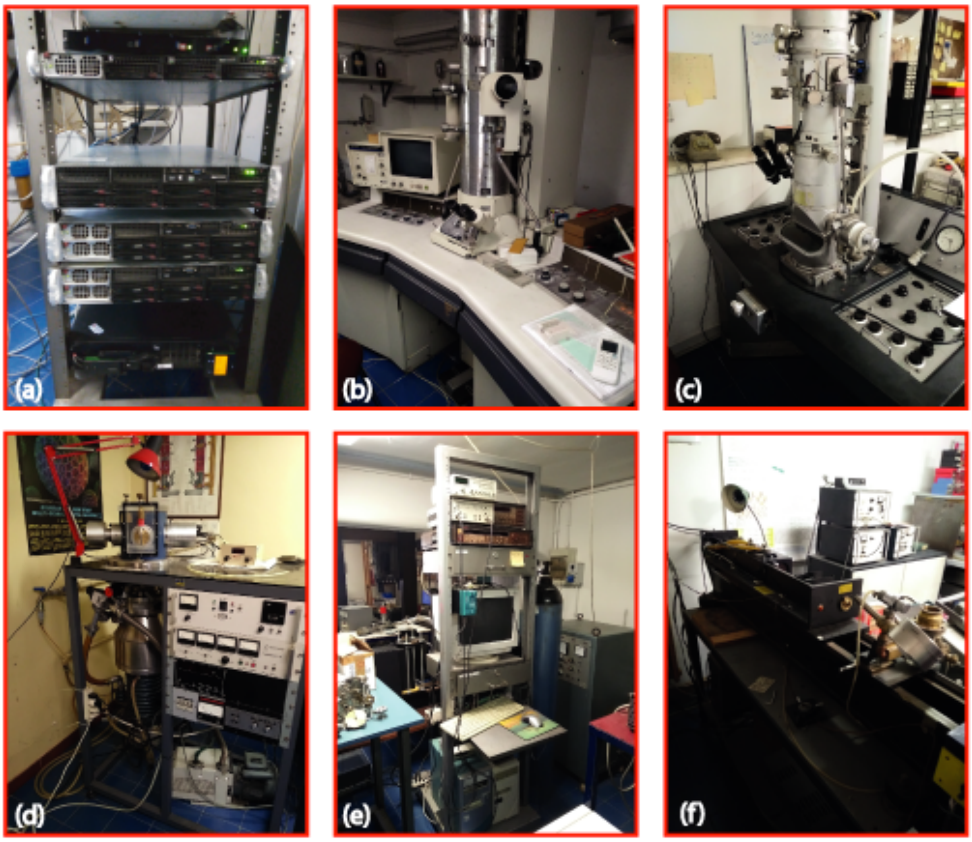


Figure 1: Some of the main apparata owned by the laboratory

The laboratory is equipped with a set-up for electrical and electronic characterisation by measuring several quantities such as the sheet resistance, the Hall voltage, the carrier density in semiconductors and thin films. The same experimental set-up has been equipped with a liquid nitrogen cryostat to perform temperature controlled measurements of the activation energy of defects and traps [Fig. **??**(e)]. With the same set-up, that is entirely controlled remotely, it is possible to perform Current Transient Spectroscopy (CTS) and Photo-Induced CTS (PICTS) measurements to study the behavior of traps and defect in semiconductors. Lastly the laboratory is equipped with a High Power Pulsed Laser system in conjunction with a controlled atmosphere system to perform experiments of laser induced modifications of the structural and the electronic properties of materials [see Fig. **??**(f)].

Physical Acoustics Lab

The Physical Acoustics Lab at SBAI Department undertakes long-term, leading-edge researches both on acoustic wave propagation in complex media, including the study of nonlinear effects, and on the interactions of acoustic waves with matter.

Research activities are primarily focussed on the following subjects:

- elastic guided waves;
- biological effects and applications of ultrasound;
- ultrasound contrast agents;
- sonoluminescence.

Lab equipment includes:

- High-frequency broadband ultrasonic pulse-echo measuring system with fourier trasform spectroscopy analysis for velocity and attenuation measurements in solid, liquid and biological samples. Attenuation spectra are measured up to 20 MHz;
- Two computer-controlled measurement systems based on optical interferometers for contactless amplitude measurement and frequency analysis of mechanical vibrations in frequency range 10 Hz - 40 MHz (displacement resolutions down to 1 nm, lateral resolution 10 μm). Vibrational amplitude map are generated with a field-of-view up to 5 cm^2;
- Network analyzer for real-time impedance measurement of ultrasound piezoelectric transducers;
- Vector Network Analyzer (VNA) for Quartz Crystal Microbalance (QCM) real time monitoring;
- Computer-controlled Quartz Crystal Microbalance (QCM) for non-invasive, label-free and highly sensitive chemical and cell biology studies with a special focus on the cell–substrate interactions. Measurements of the rheological properties of biological fluids are also carried out;
- Temperature-controlled apparatus for the study of cavitation and single-bubble sonoluminescence;
- Nd:YAG laser for photoacoustic spectroscopy measurements
- Ultrasonic transducers, power and signal amplifiers for the generation and detection of elastic waves in the frequency range 100 Hz - 25 MHz.

Figure 1: The Physical Acoustics Lab at SBAI Department

Laboratory of Radiation Protection

The Laboratory of Radiation Protection is mainly devoted to experimental applications related to environmental radioactivity (radon in air/water, radioactivity of building materials), and to nuclear measurements (alpha/beta/gamma spectrometry and neutron techniques).

Hardware:

- AlphaGUARD, for professional measurements of radon concentration in air;
- Radon chamber (founded with Sapienza grant 2017 Prot. N. RP11715C7846C2E5) for radiometric characterization of radon instrumentation in static and dynamic tests;
- Prototype for an electrostatic precipitation system designed to control radon-related potential alpha energy concentration in air as a remedial action against radon issues;
- Sodium Iodide-based gamma spectrometry systems for analyses of samples in low-background shielded well;
- High spatial-resolution tomographic system for analyses of small samples by means of a X/gamma-based automatic reconstruction system;
- Alphaino detector, designed and constructed for low-cost alpha spectrometry of samples;
- Radonino detector, designed and constructed for low-cost measurements of the radon-related potential alpha energy concentration in air (PAEC);
- 3D printer for self-building of components;

Software:

- Monte Carlo N-Particle eXtended, MCNPX, for shielding calculation, detector simulations and radiation-based techniques optimization;
- GoldSim Simulation software for radionuclide dispersion and transport through environmental pathways;
- Autocad
- Canberra suite Genie2000 and Ortec Gamma Vision software for gamma spectrometry, Figure 2;
- Matlab and Python software for data analyses.

SapienzaTerahertz

http://sapienzaterahertz.sbai.uniroma1.it/

The SapienzaTerahertz laboratory is dedicated to the R&D of spectroscopic-imaging system working within the THz range (0.1-10)THz. The system is able to perform spectrometry and imaging (in reflectance and absorbance configuration) with high frequency resolution by using state-of-the art THz technology. It allows to perform fast THz imaging analysis by exploiting a THz 2D-sensor. The system is compact allowing to perform measurement in-situ which is practical for many cultural heritage analyses, or for open field applications as the monitoring of atmospheric pollutants. The laboratory hosts two main apparatus composed by:

1st apparatus:

1) THz Quantum Cascade Laser sources emitting radiation within (1.6-5) THz at the mW level.
2) 2D microbolometer sensors (384 x 288 pixel, 35 μm pixel pitch) working at room temperature.
3) Pyroelectric sensors
4) Raster scan set-up

2nd apparatus:

Coherent THz spectrometer based on photoconductive antennas that are triggered by infrared lasers. The spectrometer allows to scan the frequency range (0.05-3) THz with resolution down to 10MHz.

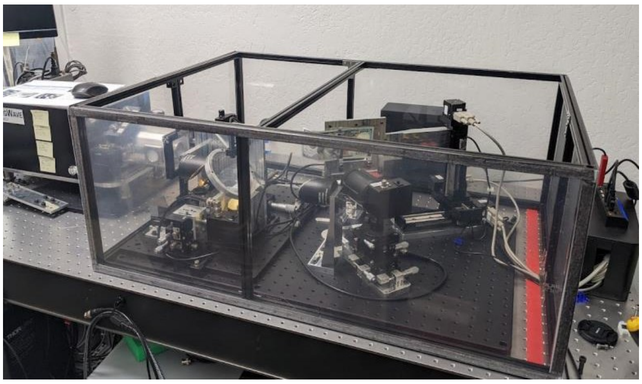


Figura 1 QCL laser source and optical set-up to perform imaging/spectroscopy in transmission and reflection. The system is contained in an atmospheric controlled box. It can be used in raster-scan configuration and/or imaging mode thanks to a 2D microbolometer camera.

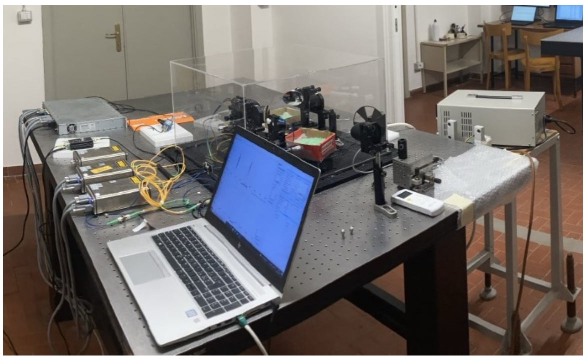


Figura 2 Spectroscopy/imaging system based on Photoconductive antennas and DFB fiber-coupled IR laser.

Fundings: "Sapienza" competitive grants: ***Grandi Attrezzature di Ateneo* & *Grandi progetti di ricerca***

Spettroscopia Laser – SpeL

The laboratory carries out research activities in the field of nanophotonics through experimental measurements of luminescence and transmission spectra in circularly polarized light. Experimental apparatuses are also being developed for the generation of second optical harmonic and for photoacoustic absorption spectra in circular light. Spectroscopy techniques are non-destructive techniques aimed at the characterization of innovative materials. In particular, the laboratory will investigate the responses of nanostructures and molecules to circularly polarized light in order to highlight particular symmetries in the materials themselves.

The spectral properties of photoluminescence light emission of coupled and uncoupled molecules in nanostructures are also currently being investigated, as well as photothermal spectral absorption measurements in circularly polarized light.

Tuneable fs laser source is available working in the 680 nm -1080 nm spectral range (Coherent), partially financed by the LASAFEM Sapienza Università di Roma Infrastructure Project prot. n. MA31715C8215A268.

Also cw UV and VIS lasers are available. Spectrometer working in the range 200nm-800nm (Hamamatsu) is available.

Figure 1. Set up for the measurements of the fluorescence detected circular dichroism on molecules deposited on nanostructures, excited by UV light.

The lab is available for PhD students training in the frame of the EU Center of Excellence ENSEMBLE3 project.

Applications:

- Measurements of circular light transmission spectra of nanostructures for different angles of incidence.
- Circular light reflection measurements of nanostructures for different angles of incidence.
- Measurements of circular light transmission spectra of molecules in solution and on nanostructured substrates.
- Measurements of luminescence spectra of molecules in solution and on nanostructured substrates under excitation of circularly polarized light.
- Photoacoustic absorption measurements in circular polarized light

Collaborations:

- University of Padua
- University of Pavia
- University of Warsaw

https://www.sbai.uniroma1.it/strutture/laboratorio_spettroscopia_laser

Laboratories for structural morphological and electrochemical materials characterization

The research activities are carried out mainly in three laboratories that are located in the building RM017 rooms 116, 120, and S09.

The scientific equipment present in the laboratory are: X-ray diffractometer, BET, Scanning Electron Microscope and Atomic Absorption, represented respectively in figure 1 a), b), c) and d) for morphological, chemical and structural characterization,

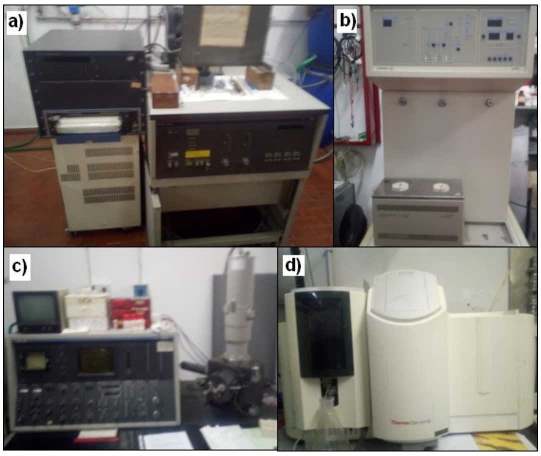


Figure 1) a) X-ray diffractometer, b) BET, c) Scanning Electron Microscope d) Atomic Absorption

ball milling, heating/stirring plates, muffles, stove, precision scales, dry-boxes, chemical hood, ultrasound bath, buki, etc. for material preparation, are instead reported, in part, in figure 2 e) and f) and finally automated devices to carry out battery charge and discharge cycles, multimeters, galvanostat-potentiostats, electrochemical impedance (Frequency Response Analyzer) for electrochemical characterization, are reported in figure 2 g) and f).

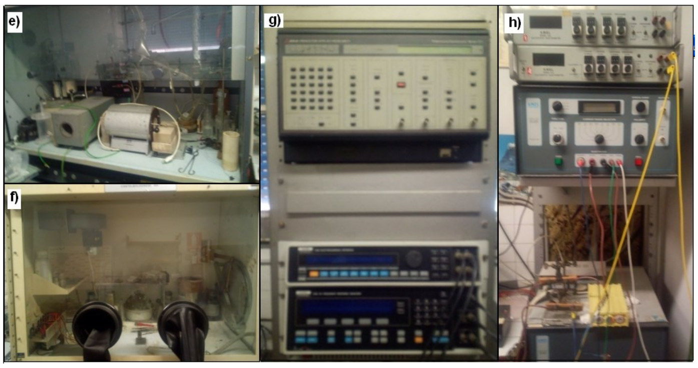


Figure 2) a) chemical hood, b) dry-boxe, c) Frequency Response Analyzer d) galvanostat-potentiostats

Laboratory of thermal analysis for characterization of materials

The research activity is carried out in the laboratory located in the Building RM017, room 1.15. The scientific apparatuses are mainly represented by the following equipments.

Figure 1) Stanton Redcroft Simultaneous Thermogravimetry and Differential Thermal Analysis (TG/DTA) equipments (STA 1500 and STA 625 models on the left and right, respectively)

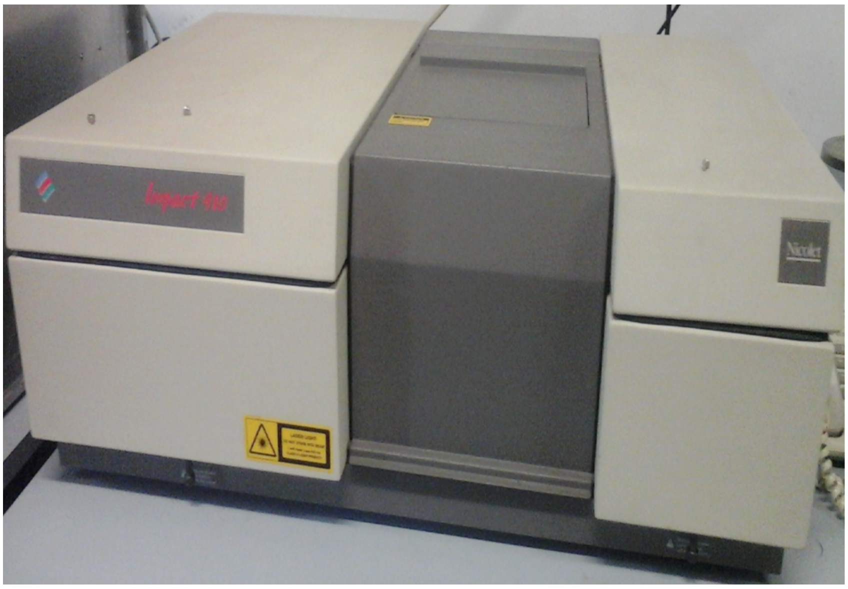


Figure 2) Nicolet Impact 410 Spectrophotometer