

**Dipartimento  
di Scienze di Base e Applicate  
per l'Ingegneria**

**Scientific Report  
2015 – 2017**

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**SAPIENZA**  
UNIVERSITÀ DI ROMA

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DIPARTIMENTO DI SCIENZE  
DI BASE E APPLICATE  
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Scientific Report 2015–2017

Edited by S. Atzeni, D. Giachetti, A. Savo, A. Schiavi and S. Vecchio Cipriotti

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## Introduction

I am very pleased to introduce the 2015–2017 Scientific Report of the Department of Basic and Applied Sciences for Engineering (Dipartimento di Scienze e di Base e Applicate per l'Ingegneria, SBAI). Our Department originated, in 2010, from merger of three previous structures, namely the Department of Mathematical Methods and Models, the Department of Energetics and the Chemistry section of the Department of Chemical Engineering, Materials and the Environment. These former entities had in common both teaching mathematics, physics and chemistry subjects for the Engineering Schools of Sapienza, and research on topics of the respective disciplines with significant application implications.

SBAI Department research activities are indeed often unique inside Sapienza, being focused on engineering applications as well as on the development of interdisciplinary diagnostic/analytical methodologies. The wide spectrum of such activities is well represented by the one-page reports on about 60 research lines, that make the core of this report, and are grouped in the subject areas of Chemistry, Mathematics and Physics.

In addition to caring of most of the basic sciences teaching for undergraduate and Master courses of the Sapienza Schools of Engineering (with about 2000 new students a year), the Department is managing the (International) Master Course on Engineering Nanotechnology. Another important activity, just connecting teaching and research, is the Department's Ph.D. in Mathematical Models for Engineering, Electromagnetics and Nanosciences. Furthermore, quite a few members of the Department participate in the Board (and supervise most of the students) of the Ph.D. Course in Accelerator Physics, formally hosted by the Department of Physics.

The reports also presents short descriptions of Department's facilities, laboratories in particular, where a large part of the researches presented here were performed. The long list of publications, as well as of grants, which conclude the report, also testify the quality of SBAI research and its positioning within the international scientific community.

In conclusion, I would like to thank all scientists who contribute to the healthy scientific life of the department, and all the administrative and technical staff, for their invaluable support.

Luigi Palumbo

Director



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# Research Activities: Chemistry

# Chemistry - Introduction

SBAI research in Chemistry covers a few wide, and in some cases interconnecting, areas of the Chemical Fundamentals of Technologies that characterize both teaching and research activity of each chemist.

The following one-page summaries show how SBAI chemists combine their expertise in chemical fundamentals (the basic topic taught for the School of Civil and Industrial Engineering), with some of the most attractive and promising applications mainly related materials sciences. These can be listed as follows: applied electrochemistry (concerning materials for batteries or organics for electronics, production of hydrogen, antioxidant properties of phenolic compounds), ionic liquids (as solvents, or electrochemical precursors, or to analyze the competition between vaporization and decomposition), materials science, thermal behavior of materials.

Instrumental to the above researches is the in-house availability of a number of diagnostic techniques, including X-ray Diffraction Powders, Scanning Electron Microscopy, UV-Vis, NMR and FTIR spectroscopies, Liquid Chromatography (LC)) coupled to Mass Spectrometry (MS), Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry). Our laboratories are also available for collaboration with external users. A few researches have been performed in collaboration with groups belonging to other national or foreign research institutes. Among them, Consiglio Nazionale delle Ricerche (CNR) and Centro Ricerche Casaccia of Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile (ENEA), deserve to be mentioned.

In particular, during the period 2015–2017, SBAI chemists focused their efforts to apply electrochemistry to leading topics like ionic liquids and the production and storage of energy, lithium-ion batteries, chemical synthesis of organic materials for electronics, redox properties of potential antioxidants. Other pursued research areas include electrochemical synthesis of nanostructured materials for energy applications, and the study of thermal behavior of materials (gel-glasses and organic-inorganic hybrids, waste plastics, oxidized olive and essential oils, imidazolium ionic liquids).

# Chemistry - List of research activities

- C-1. Structural, morphological, and electrochemical materials characterization
- C-2. Electrochemistry in/of ionic liquids
- C-3. Carbon dioxide in organic synthesis: organic carbamates of industrial interest
- C-4. New compounds for organic electronics
- C-5. Applied electrochemistry
- C-6. Antioxidants, an all-round view: from electrochemistry to agro-food matrices
- C-7. Thermal behaviour and thermal stability of different classes of materials

## C-1. Structural, morphological, and electrochemical materials characterization

*A. Dell'Era, M. Pasquali, F. Scaramuzzo, S. Vecchio Cipriotti*

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

**Recycling of batteries.** Heavy metal electrodeposition studies have been carried out and are carried out through a cell with three-dimensional RVC electrodes (reticulated vitreous carbon), which is then used as an electrochemical filter of sulfuric lye solutions of the cathode material of spent batteries. The process is studied not only for the recovery but also for the removal of heavy metals present as pollutants in wastewater such as Ni, Pb, Cr as well as Co.

**Unconventional electrochemical systems for energy production and storage.** The study consists of researching cathode materials for lithium ion and lithium-ion batteries. Materials for this purpose are  $\text{LiMn}_2\text{O}_4$ ,  $\text{LiNiO}_2$ ,  $\text{LiCoO}_2$  and  $\text{LiFePO}_4$  as well as more or less amorphous charcoal graphite, silicon, perovskites, titania etc. The materials are characterized structurally, [1] morphologically and electrochemically. These characterizations are essential especially for automotive applications for determining the parameters crucial for the proper functioning of BMS systems.

**Morphological-structural investigations of electrode and non-electrode materials.** Lithium intercalation mechanisms in 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 X-ray analysis of samples with various degrees of intercalation. In this research topic, electron microscopic analyses are also carried out to observe the morphology of the cathodic powders and to determine the influence it has on 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 [2] such as, for example, the absorption and desorption of hydrogen [3].

**Electrochemical production of hydrogen.** This study is focused in the research of new electrode materials whose production processes are simple, inex-

pensive and with good catalytic activity. The electrode materials that are the object of our study are binary and ternary Ni-Co alloys [4] prepared electrochemically by deposition with constant current and with controlled potential on metal foils or meshes. Morphological-structural investigations are performed using XRD and SEM. while the electrochemical characterization of the electrodes is made by measuring the exchange current density and the overvoltage discharge of hydrogen and oxygen in an electrochemical cell.

**Photo-assisted electrolysis.** Titanium dioxide has already been used as a photocatalyst; it is non-toxic, stable and inexpensive. By using simple electrochemical techniques, in our laboratory we prepared a photo anode of  $\text{TiO}_2$  nanotubes able to give photocurrent values three times higher than those normally reported in literature [5]. The high reaction yield brings this new material closer to others that are currently undergoing industrial experimentation.

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5. F. A. Scaramuzzo *et al.*, Journal of Applied Electrochemistry **45** 727 (2015).

## C-2. Electrochemistry in/of ionic liquids

I. Chiarotto, M. Di Pilato, M. Feroci

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 physicochemical properties their use is advantageous in view of a *greener* way of thinking Chemistry although there are not sufficient studies on their possible toxicity. 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 procedures 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 strong bases, but can also be carried out by cathodic reduction [1] (See Fig. 1).

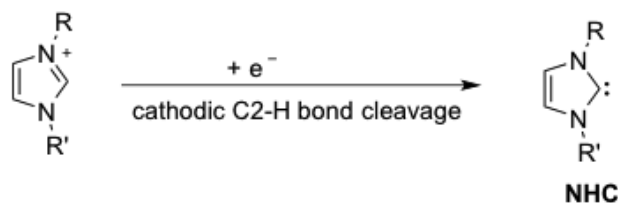


Figure 1: Electrochemical generation of NHC.

The advantages of the electrochemical deprotonation are the easiness of controlling the amount of reagent by simple control of the current, the "greenness" 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. But the electrochemical methodology has also the advantage of being able to quantify the amount of NHC simply recording a cyclic voltammetry (Fig. 2). In fact, NHC obtained by cathodic reduction of the imidazolium cation ( $\text{BMIm}^+$ ) can be oxidised at a potential near 0 and its concentration is proportional to the peak current corresponding to this oxidation [2]. The efficiency of NHC electrochemical generation and its stability depend on the structure of the imidazolium cation and on the presence, in solution, of reagents and impurities. [3] In some cases, when the basicity of imidazolium ionic liquid anion is sufficient, NHC can be spontaneously present in pure ionic liquid, in an amount which is dependent also on the temperature. 1-Butyl-3-methylimidazolium acetate is an example of such NHC containing ionic liquids, and

again the presence of NHC can be put in light using cyclic voltammetry [4].

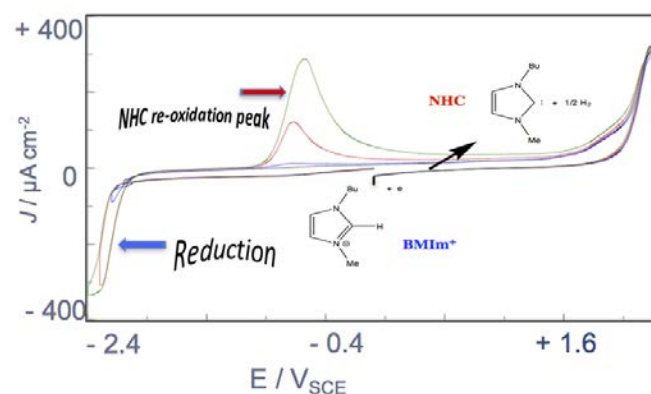


Figure 2: Cyclic voltammetry of  $\text{BMIm-BF}_4$ .

### References

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### C-3. Carbon dioxide in organic synthesis: organic carbamates of industrial interest

*M. Feroci, I. Chiarotto, M. Di Pilato*

Carbon dioxide is regarded as the primary anthropogenic contribution to the greenhouse effect. Resources spent on strategies that limit the release of carbon dioxide into the environment have considerably increased during last decades. However, CO<sub>2</sub> represents a cheap and readily accessible carbon source, but it is characterized by a notably inert nature. Methods to overcome this inertness generally require harsh reaction conditions, such as high pressure or the presence of strong nucleophiles, and appear quite cumbersome to operate on a large scale. Most importantly, they often make use of metal catalysis, raising concerns on the environmental impact of waste management.

Carbon dioxide can be activated under very mild conditions by cathodic reduction. The electrolysis cell is very simple, and can operate in open vessel (Fig. 1). If after cathodic reduction an amine and then an alkylating agent are added to the mixture, very high yields of the corresponding dicarbamates can be obtained (Fig. 2) [1,2].

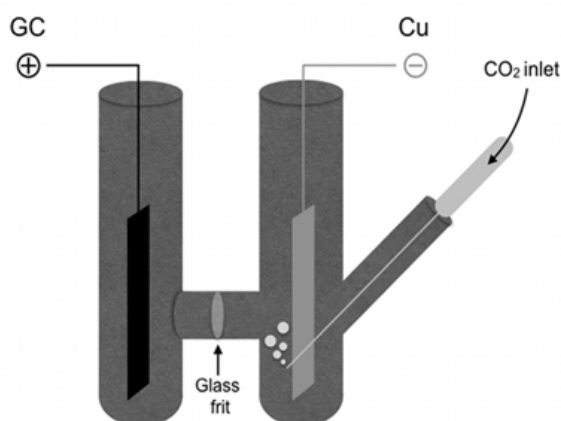


Figure 1: Electrochemical cell for CO<sub>2</sub> reduction.

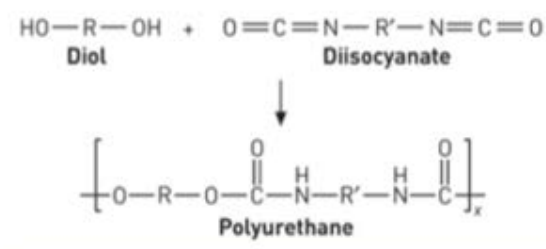


Figure 2: Synthesis of polyurethanes.

Moreover, dicarbamates can be obtained from diamines by reaction with tetraalkylammonium hydrogen

carbonate, in a very sustainable organic synthesis [3,4]. In this case, the reagent can be easily recovered, regenerated and reused multiple times, rendering this synthesis advantageous also from an industrial point of view.

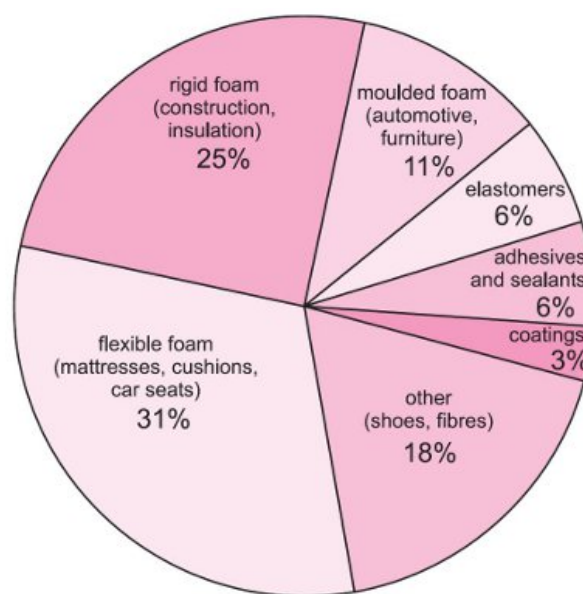


Figure 3: Polyurethane uses.

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2. G Forte et al., *React. Chem. Eng.* **2** 646 (2017).
3. International patent. Inventors: I. Chiarotto, M. Feroci, G. Forte, A. Inesi, F. Richter, V. Trieu "Sustainable Synthesis of carbamate compounds" Applicant: Covestro AG (De). Publication number: WO2017/137343 A1. Publication date: 17.08.2017.
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## C-4. New compounds for organic electronics

*L. Mattiello*

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 comprises several applications, e.g.: Organic Light-Emitting Diodes (OLED), Organic Photovoltaics [1,3], Intramolecular Charge-Transfer Sensors, Organic Field-Effect Transistors, Organic Photodetectors, Terahertz Organic Crystals, Photonic Integrated Circuits (PICs) [2,4], Organic Scintillators, and many more. In the domain of organic semiconductors, several thiophene derivatives were newly synthesized and fully characterized, both from an experimental point of view (physico-chemical, electrochemical, optical) and with a computational approach [3].

Despite the fact that polythiophenes were the first and most used thiophene derivatives, they suffer from several points of view (e.g.: the lack of well-defined chemical structures, the presence of impurities and the presence of defects in molecular structures) whereas a high grade of purity and synthetic reproducibility are requested, in order to clearly address the syntheses of materials with precise and specific properties. In this respect, oligothiophene molecules represent the perfect compromise between purity and performance. They can be regarded either as model compounds for the study of structure-property relationships relative to polythiophenes, and as self-consistent materials that can possess unique and superior characteristics (physico-chemical, optical, electronic, self-assembly properties, possibility to work in solution, ease of purification, low-cost synthetic procedures, and so on) over their polymeric counterparts.

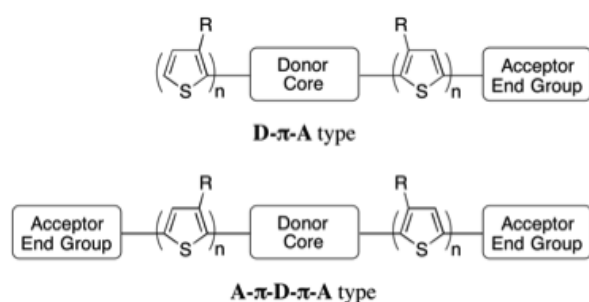


Figure 1: D- $\pi$ -A and A- $\pi$ -D- $\pi$ -A molecular architectures of newly synthesized oligothiophenes.

As an example, in the field of Organic Photovoltaics, dipolar push-pull chromophores with highly polarizable  $\pi$ -electron systems with donor (D) and acceptor (A) groups possess properties that result from the existence of photoinduced intramolecular charge transfers at quite low energies. Among small molecules, thiophene oligomers possess extended  $\pi$ -electron delocaliza-

tion along the backbone and are good hole-transporting materials. The newly synthesized oligothiophenes possess low bandgaps, a condition required for their applications in several fields of Organic Electronics, and there are also clear evidences that they represent promising candidates for future studies directed to fine-tune their optical, electrochemical and morphological properties in order to satisfy the requirements coming from the different fields of application of organic semiconductors.



Figure 2: chloroform solutions of oligothiophenes (1 mM); UV light illumination at 254 nm (left) and at 365 nm (right).

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## C-5. Applied electrochemistry

*M. Pasquali, A. Dell'Era, F. Scaramuzzo, M. Ottaviani*

### Lithium batteries and lithium ion batteries.

This research field includes various topics which are listed below: - Synthesis of cathode materials able to intercalate  $\text{Li}^+$  ion within their crystalline structure.

- Thermodynamics of the intercalation of alkaline ions in transition metal oxides. These studies are carried out on a thermodynamic basis for the determination of intercalation enthalpies with calorimetric techniques. Moreover, potential spectroscopy is used in order to determine the variation of intercalation free energy and the distribution of ions in the crystalline structure during intercalation, which is correlated to the entropic state of the system.

- Intercalation kinetics. The aim of this study is to determine the diffusion coefficients of the  $\text{Li}^+$  ion. For this purpose, electrochemical techniques such as galvanostatic impulse or impedance measurements are used.

- Structural investigations on solid solutions of transition metal oxide compounds; We start from the determination of the crystallographic parameters of the starting materials, and we observe their variations during the intercalation process. In this way the maximum intercalation limit of the  $\text{Li}^+$  ion is established avoiding irreversible modifications of the structure. This research is carried out by XRD and SEM analyses and the surface area developed by these materials is measured by BET technique.

- Characterization of electrolyte solutions. Due to the nature of the anode, lithium and lithium-ions batteries require the use of organic electrolytes or liquid ionics. In this context, we study the stability of different electrolytic solutions with the various electrode materials used by means of impedance measurements. In this way we are able to determine the characteristic of the electrical double layer at the electrode/solution interface both on the lithium and on the cathode.

- Li ion cells; In this case we use graphite or carbon directly with a material that can supply  $\text{Li}^+$  ions. Suitable materials are  $\text{LiMn}_2\text{O}_4$ ,  $\text{LiNiO}_2$ ,  $\text{LiCoO}_2$  and  $\text{LiFePO}_4$ . In order to obtain batteries with greater capacity, recently, the use of Ti nanotubes [1] and Si nanowires as anode and lithium sulphide as cathodes are being studied [1].

### Fuel Cells and Li/air Batteries.

Nanostructured electrocatalysts for fuel cells and Li/air batteries. The aim of the study is to find the optimal conditions of synthesis by electrocrystallization of platinum nanoparticles to be used as catalyst on various carbon substrates including nanotubes. The resulting materials can be used as electrodes in polymeric or direct methanol fuel cells as well as in electrolyzers and lithium/air

batteries. The work aims to optimize the electrodeposition methodology to have a high catalytic activity. The goal is to have the best electrode materials with low platinum load. For this purpose, electrochemical techniques such as galvanostatic deposition (single and multiple impulse) were used, defining the operative parameters that allow to obtain nanostructured materials with high electrocatalytic activity. The electrode materials suitable for this purpose must possess the following features: high specific surface, good electrical conductivity, low hydrogen over-voltage, selectivity, electrocatalytic behavior, and low cost. Our study is focused on the research of new electrode materials, which are at the same time easy to prepare, inexpensive and characterized by a good catalytic activity. The electrode materials of our interest are binary and ternary alloys based on Ni-Co-Mo prepared by means of electrochemical deposition on metal foils or meshes at constant current and/or controlled potential. The use of the two electrochemical techniques leads to deposits with different composition and morphology.

**Hydrogen production.** Finally, the photoelectrochemical production of hydrogen by direct splitting of water involves the use of semiconductors. A good material for photocatalysis must have [3]: an appropriate band gap between the conduction and valence bands for the splitting of water (approximately 2 eV), an optical absorption in the visible and ultraviolet spectral regions, good stability in electrolyte solutions and a good efficiency in charge transfer between the semiconductor and the electrolyte. Titanium dioxide has already been used as a photocatalyst; it is non-toxic, stable and inexpensive. By using simple electrochemical techniques, in our laboratory we prepared a photoanode of  $\text{TiO}_2$  nanotubes able to give photocurrent values three times higher than those normally reported in literature. The high reaction yield brings this new material closer to others that are currently undergoing industrial experimentation.

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## C-6. Antioxidants, an all-round view: from electrochemistry to agro-food matrices

R. Petrucci

The well-known beneficial health effects associated with a diet rich in fruits and vegetables have been attributed in part to the antioxidant properties of phenolic compounds widely distributed in dietary plants. The antioxidant capacity of phenolic compounds tested *in vitro* is widely reported in literature, as also pro-oxidant effects, evidenced by some other tests. Conversely, mechanisms involved in the complex chemistry of the so called antioxidants are still far to be understood, and studies on the reactivity of given compounds, in terms of molecular mechanism, are still required [1].

My research activity ranges in the field of antioxidants and focuses on two major topics:

- molecular electrochemistry of potential antioxidants, to study redox properties, oxidative mechanisms and structure-activity relationship (SAR);
- analysis and characterization of agro-food products, wastes and by-products, by chromatographic separation and mass spectrometry.

In particular, in the last three years:

- the oxidative mechanism of caffeine, recently suggested as an antioxidant, was studied by spectro-electrochemistry and theoretical calculation [2] (Fig. 1). The study was carried out in collaboration with Giuseppe Zollo, researcher of SBAI.

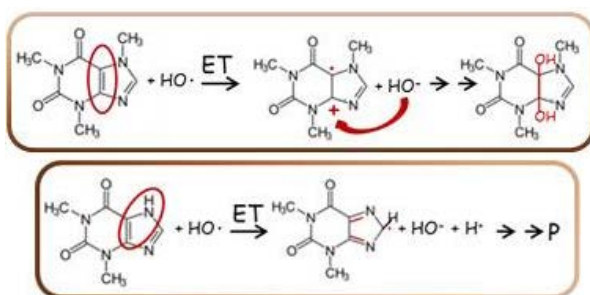


Figure 1: Oxidative mechanism of caffeine.

An electrochemical sensor highly selective for the determination of caffeine was developed and tested on real matrices [3] (Fig.2). The study was carried out in collaboration with Antonella Curulli, CNR researcher guest at SBAI.

- The metabolic fingerprinting of *A. pungens* and *A. uva-ursi* leaf extracts was carried out by UHPLC-PDA-TOF/MS analysis and main differences were found. Markers for *A. pungens* were found, to identify samples marketed as *A. uva-ursi* [4] (Fig. 3).

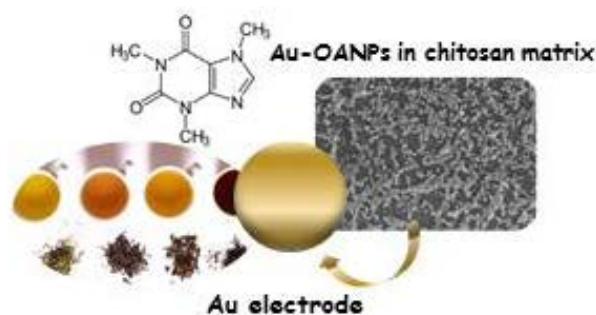


Figure 2: Sensor for caffeine.

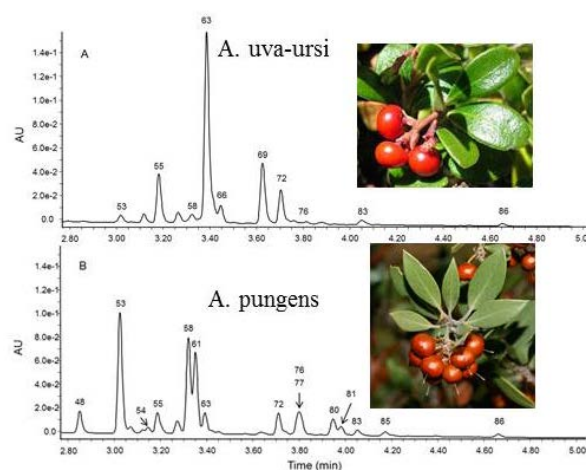


Figure 3: Identification of markers of *A. uva-ursi* and *A. pungens*

The study was carried out in collaboration with Istituto Superiore di Sanità (ISS).

The metabolic profiling of arabica and robusta coffee silverskin, was carried out by UHPLC-PDA-TOF/MS. Differences in the metabolites distribution, polyphenols contents and antioxidant capacity were found. The content of antioxidants and phytochemicals were compared, the suitability of silverskin as a functional food ingredient evaluated ([5], in collaboration with ISS and DICMA).

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## C-7. Thermal behaviour and thermal stability of different classes of materials

*S. Vecchio Cipriotti*

The knowledge of thermal behavior is of crucial importance for several classes of materials because of the occurrence of fire accidents, or since they have been placed in stores, where very hot temperatures can be reached especially during the summer. On the other hand, in some cases materials defined as precursors were treated at defined high temperatures to cause specific properties or to increase other (metals increase their mechanical properties upon heating). So, thermal analysis techniques offer the possibility to study 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. To this end a powder sample is subjected to a temperature program (usually heating at constant rate) under a controlled atmosphere of a purging gas.

My research has been focused on material science with particular reference to the thermal behavior study of different classes of materials, like: halloysite nanotubes, gel-glasses and organic-inorganic hybrids (OIHs), waste plastics, oxidized olive and essential oils, imidazolium ionic liquids [1–5]. 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).

In particular, pristine and modified halloysite nanotubes (the latter was treated by acidic solution to cause a significant increase of the tube lumen) underwent dehydration and dehydroxylation upon heating and the results of kinetic analysis of both processes were compared with those of kaolinite and explained in terms of the strengths of the hydrogen bonds broken.

The thermal behavior of silica-based gel glasses or silica- and zirconia-based OIHs with polyethylene glycol (PEG) as the organic component was studied with the view to find the most suitable temperatures for the thermal treatment to improve their properties. Morphological and structural properties were also studied by scanning electron microscopy and X-ray diffraction analysis. 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 etheral oxygen atoms (H-bond acceptors) or terminal -OH of the PEG 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.

Among the techniques used to study oxidation in olive oil, thermal analysis (TA) provides useful information about the thermal behavior of the samples as affected by oxidation. The DSC curves of olive oil, both on cooling and heating, has been found to be largely influenced by the oxidative status of the samples and different statistical approaches have been successfully proposed to correlate the thermal parameters with the conventional chemical indicators of oxidation. DSC can be also used to study the kinetics of phase transition phenomena as affected by oxidation. Vaporization studies performed using effusion Knudsen and thermal analysis techniques have also been aimed at measuring the evaporation enthalpy for the more fundamental purpose of evaluating the cohesion energy in the liquid phase, so as to adjust/validate force field parameters for molecular dynamics calculations. Nevertheless, absolute vapor pressure data for ILs 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. Our multitechnique approach used two techniques based on molecular effusion under reduced pressure (under Knudsen regime) aimed at studying the competition between simple evaporation and thermal decomposition of imidazolium ionic liquid BMImPF<sub>6</sub>.

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# Research Activities: Mathematics

# Mathematics - Introduction

There is a deep connection between partial differential equations (PDE's) along with their discrete, numerical or probabilistic versions, and differential geometry or mathematical physics. Many physical principles are governed by variational principles; Euler made the statement that *...nothing at all takes place in the universe in which some rule of the maximum or minimum does not appear*. In this case, when the maximum or the minimum is achieved (for example, when potential energy is minimized), the physical law is also described by a partial differential equation, the Euler-Lagrange equation. At the same time, physical laws often have a purely geometric description : Einstein's field equations of General Relativity involve the Ricci curvature tensor of space-time; the constancy of the mean curvature is the Euler-Lagrange equation for the minimization of surface area. On the other hand, the symmetries of a physical system, from both discrete and continuous aspects, can be described and understood by representation theory of groups and algebras.

These connections are particularly evident in our department, where researchers often interact to analyze the same problem from different points of view. We loosely identified some of the research themes below.

## **Diffusion in composite materials or irregular structures (M-1 to M-13)**

Composite materials are playing nowadays an increasing role due to the fact that they have a wide spectrum of applications in material sciences and in medical processes. For example, this is the case for diffusion in biological tissues, where a large number of microstructures, assumed to be disposed in a periodic array and separated by active interfaces, are present. Composite materials are obtained finely mixing two or more components according to a very small positive parameter which will go to zero. This process, which starts from a microscopic description of the problem and provides at the end a macroscopic, effective representation of it, is called homogenization.

Due to the presence of microstructures and interfaces between them, the mathematical modeling of diffusion throughout composite materials requires a complex PDE's approach which often induces challenges of geometrical and numerical nature; in particular, for wave propagation in porous media the PDE could be of fractional order.

On the other hand diffusion phenomena can take place across irregular media having nevertheless fractal properties i.e. self-similarity properties, like sprays in the lungs or diffusion processes in physiological membranes. Fractal interfaces are also considered in diffusion processes in which we want to enhance the absorption effects of the layer by increasing its surface and preserving small volumes. Moreover there are many situations where the system evolves along networks, which of course can be considered as irregular structures. This happens for example in neurobiology, data transmission, traffic management problems, crowd motion or consensus formation where the system is a complex system which means that it is composed by a large number of agents with decision abilities and objectives. In many of such situations we need to develop new decision models under uncertainty and ambiguity.

## **Discrete geometry and representation theory (M-14 to M-18)**

It is common in many applications to reduce a continuous model to a discrete one which will make calculation more approachable; in fact, this is one of the scopes of numerical analysis. But there are other reasons why discrete mathematics has so many applications, and many concepts in mathematics have a discrete counterpart: for example, discrete geometry and graph theory which, in turn, have fruitful connections with other fields of mathematics. Enumeration of a finite set of objects with respect to a given set of restrictions leads to extremal combinatorics, which can be approached through algebraic varieties over finite fields; the search for graphs which optimize some

properties of edge-colouring is another example of such instances. Orthogonal polynomials show up, sometimes unexpectedly, in many kind of computational problems, including special functions, matrix theory and combinatorics. Quivers are special oriented graphs which have connections with algebra and Lie theory; the classification of their representations is an active field of research which recently has been approached with more geometric tools (quiver Grassmannians).

### **Harmonic analysis and operator algebras (M-19 and 20)**

In harmonic analysis a function is represented as a sum of its Fourier series, and then it can be decomposed into a superposition of simpler eigenmodes. This idea has had enormous impact on practically all applied sciences; what matters to us here are its discrete and non-commutative versions. The first has applications to graphs and finite groups; in the second, which has deep applications to mathematical physics, the basic idea is to move from the abelian case to groups which are neither compact nor commutative (e.g. Lie groups or algebraic groups). Gelfand pairs is a unifying concept between the commutative and the non-commutative case.

### **Evolution models, inverse problems and stochastic phenomena (M-21 to M-27)**

Following the evolution in time of a given system, we could be interested in its controllability, in its asymptotic behaviour for large time or else in the evolution of free boundaries and scaling laws. The problem of controllability of a system is of great interest in discrete and continuous models for hyper-redundant architecture, dealing with new forms of robot locomotion and grasping. Expansions in non-integer bases and Fourier method are in fact used in order to develop controllability and observability. Control and inverse problems for isotropic and anisotropic materials lead to study integro-differential equations: this kind of equations appears also in viscoelasticity and it models materials with memory, i.e. materials whose mechanical and/or thermodynamical behaviour depends also on the past times.

Image reconstruction from an empiric set of data is also an inverse problem which is always difficult to solve, and which can be usefully approached by efficient computational algorithms, the technical applications of which are quite evident. Particular attention is recently given to reconstruct deep brain activity and to study image processing connected to human vision.

Another interesting problem is the study of asymptotics and correct length-scale in thin-film equation which models the height of a droplet spreading over a substrate in wetting phenomena. Flux-saturated diffusion equations find application when a saturation mechanism appears at high gradients of the solutions. In this case the study of propagation of solution's support and waiting time phenomena are interesting questions from the point of view of applications.

Particle flows in presence of obstacles is another research line which is of great interest in Statistical Mechanics and Stochastic Particle System. Obstacles can reduce or accelerate the dynamics, giving rise to anomalous diffusions like in cells where macromolecules play the role of obstacles for smaller molecules.

### **Partial differential equations in Geometry and Physics (M-28 and 29)**

In many problems of applied sciences modeled by partial differential equations one observes the formation of geometric structures as a parameter approaches a singular value. In order to understand these phenomena a key issue is to identify an associated singular limit problem and to investigate its solution structure, which can be an autonomous partial differential equation or system in entire space; research then focuses on nonlinear elliptic equations and systems, including local and nonlocal ones whose common patterns are concentration phenomena, like nonlinear Schrödinger equations and prescribing scalar curvature problems, for example, the Yamabe problem.

The analytic methods connected to the theory of PDE's are effective tools to understand geometry and mathematical physics, and there is a deep interplay between geometric structures of manifolds and spectra of various elliptic operators, which is one direction of the research in differential geometry at our department.

# Mathematics - List of research activities

- M-1. Homogenization techniques in biological tissues
- M-2. Multiscale models and computational methods for image processing
- M-3. Mathematical models for interacting systems on networks (MathNets)
- M-4. Fractional and anomalous diffusions on fractals
- M-5. Fractional Derivatives and non linear dynamics
- M-6. Anzellotti's pairing theory and applications
- M-7. Homogenization for singular semilinear elliptic problems
- M-8. Interfaces and scaling laws in nonlinear PDEs
- M-9. Fast diffusion across fractal interfaces
- M-10. Singular elliptic Dirichlet problems
- M-11. Numerical solution of fractional differential equations
- M-12. Decision models under ambiguity
- M-13. Boundary value problems in irregular structures
- M-14. Algebraic and combinatorial aspects of orthogonal polynomials, hyperbolic polynomials, finite fields
- M-15. Geometric methods in representation theory of finite dimensional algebras
- M-16. Umbral calculus
- M-17. Finite geometry and combinatorics
- M-18. Graph colouring and graph labelling: some connections with geometry and algebra
- M-19. The world of  $C^*$ -algebras: general aspects and applications to Quantum Field Theory
- M-20. Discrete harmonic analysis and representation theory
- M-21. Asymptotic behavior for nonlinear parabolic equations
- M-22. Integro-differential models & materials with memory: viscoelasticity and magneto-viscoelasticity
- M-23. Effects of spatial heterogeneities on mass transport
- M-24. Controllability of evolutive equations
- M-25. Bäcklund transformations & nonlinear operator equations on Banach spaces: structural properties and applications
- M-26. Brain Imaging by MEG/EEG data
- M-27. Integro-differential equations: well-posedness and controllability
- M-28. Perturbative methods and concentration phenomena in nonlinear problems
- M-29. Spectral and geometric analysis on Riemannian manifolds

## M-1. Homogenization techniques in biological tissues

*M. Amar, D. Andreucci*

The study of thermal, mechanical and electrical properties of composite materials plays an increasingly important role in material sciences due to the fact that these composites have a wide spectrum of applications in industrial and in medical processes. The properties of these materials are often grounded on the interplay of phenomena which take place at different space and time scales. In particular, our research focuses on problems of electrical conduction or ions diffusion in biological tissues, where a large number of microstructures, assumed to be disposed in a periodic array and separated by active interfaces, are present. These are inherently difficult subjects for mathematical modeling, since the microstructure itself (and even more the presence of interfaces), while often essential in determining the features of interest, poses an intrinsic challenge of geometrical and therefore numerical complexity. Theoretical and also applied mathematics developed the well known device of homogenization which, preserving a particular regard to scale effects, permits to simplify such schemes, making them amenable to numerical approximations.

Our research has been mainly concentrated on the following two fields of interest.

- Electrical conduction in biological tissues: there are several applications of electric potentials in diagnostic devices to investigate the properties of biological tissues. For instance, electrical impedance measurements can be employed as a non-destructive analysis tool in medical diagnostics. Such techniques are essentially based on the possibility of determining the physiological properties of a living body by means of the knowledge of its electrical resistance. However, it has been observed that, applying high frequency alternating potentials to the body, a capacitive behaviour takes place, due to the electric polarization at the interface of the cell membranes. In this regards, the biological tissue is modelled as a composite media with a periodic microscopic structure made by two finely mixed phases (intra and extra cellular) separated by an imperfect interface (cellular membrane). In particular, we considered cases where strong non-linearities appear in the model, more exactly in the resistive component of the interfacial dynamics. Occurrences of typical non-linear behaviour arise for example in the modeling of the cardiac tissue, and they are due to the biochemical properties of the cell membranes. In order to pass from the microscopic model to the macroscopic behaviour of the tissue, the homogenization theory seems to be the appropriate tool. A relevant feature of the model thus obtained is its capability of connecting the coefficients appearing in it to the physical properties of the microstructure (that is in this

case, of the cells, of their membranes, and of extra cellular space). This is particularly noteworthy when the long time behaviour of our model is analysed. In this case, as it is usually done in diagnostic, a periodic boundary data is assigned and the asymptotic behaviour of the solutions of the model is investigated under suitable assumptions on the non-linearity.

- Alternating interface conditions on cell membranes: there are experimental evidence that ionic channels form selective pores in the cell membrane which open and close allowing permeation of ions; however, the selection process of a species in the ion conduction (known as gating) is very delicate and not yet completely understood. We studied this process and proposed, as a first possible approach, that this phenomenon is modelled as a diffusion problem in a domain with holes, where the holes represent the pores which periodically and simultaneously cycle through open and closed phases. The gating in this still pioneer model is obtained choosing smaller and smaller the corresponding diffusivity in a suitably small region in the neighborhood of the holes. Assuming a very large number of very small pores (with respect to the dimensions of the domain) and taking into account also that the period of the cycle is much smaller than the characteristic time of diffusion, it is possible to approximate the microscopic model with its homogenized version, where the number of pores and the number of cycles both diverge to infinity and the diffusion in the affinity region goes to zero.

In order to achieve this result, a preliminary deepening in homogenization theory for parabolic equations with time-oscillating coefficient has been needed.

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## M-2. Multiscale models and computational methods for image processing

*V. Bruni*

The research activity mainly focused on modeling the relationships between some basic concepts of information theory and the mechanisms regulating human visual system (HVS) and on their use in the definition of efficient computational methods for the solution of some image processing problems.

**Motivation** As the final receiver of image informative content is human eye, in the last decades the need for new metrics that are able to better correlate with human perception has been increasingly evident in several applications. As a result, vision mechanisms can be used for both coding and learning image content, promoting the selection of the most appropriate model in different problems. For example, several neurological studies show that very few points in the image are able to attract visual attention in the pre-attentive phase. These points are not random and are foveated, i.e. human attention diminishes as one moves away from them. Hence, despite the multiscale nature of vision, human eye employs a resolution that depends on both spatial and spectral scene content, making linear multiscale transforms not adequate for an accurate modeling of human vision.

**Main results** The research activity within this topic has concerned:

- the formal estimation of the just noticeable detection threshold, which is related to the contrast sensitivity of human eye, and the definition of a multiscale transform with non constant and perception-based scale dilation parameter. These formal results have been exploited for defining and/or improving computational methods for image regularization, as for example image denoising, deblurring and color quantization — an example concerning denoising [1] is in Fig. 1;
- the development of a computational method for image quality assessment based on the Asymptotic Equipartition Property. It relies on a formal characterization of fixation points in the pre-attentive vision as the typical set of the metric used for quality assessment. The typical set depends on the image distortion kind. Based on this model, a computationally efficient iterative algorithm for the extraction of a sequence in the typical set has also been developed and a criterion for the stopping rule has been provided. Experimental results show that image quality can be assessed with high accuracy using less than 10% of image pixels — an example concerning the structural similarity index (SSIM) for blurred images [2] is in Fig. 2;
- the modeling of some neurological evidences re-

garding the statistical independence of luminance and contrast in correspondence to fixation points and their use for the improvement of computational methods for target tracking in video sequences. The resulting algorithms are computationally efficient and robust to occlusions and luminance changes and have been successfully applied in videosurveillance and biometric applications — an example concerning iris tracking [3] is in Fig. 3.



Figure 1: Noisy image (left): noise is not perceived on the rocks. Conventional regularization (middle):- rocks texture is oversmoothed. Perception-based regularization (right): rock texture is preserved.



Figure 2: Original (left) and blurred image (middle). Selected fixation points (right).



Figure 3: 8 frames of a video sequence. The tracker is robust to eye blinks and iris movement.

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## M-3. Mathematical models for interacting systems on networks (MathNets)

*F. Camilli*

The aim of the research is to study 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 Economy and Biology since they pose new and stimulating scientific challenges with respect to more traditional systems: "Today, most of science is biology" [1] and also in Mathematics biological applications are becoming the main driving force of innovation.

Living complex systems are composed by a large number of agents who have some decisional abilities and objectives. From this point of view they differ from particle systems in Statistical Mechanics, where a single individual follows prescribed motion rules. As consequence the collective behaviour of these systems is more complex than the simple superposition of individual actions and for its comprehension is necessary to pursue new mathematical methods.

In many situations, complex systems evolve on irregular spatial domains such as networks and fractal sets. Indeed network structures are ubiquitous in the real world and are at the frontier of applied mathematics. They arise in a natural way in data transmission, traffic management, crowd motion, consensus formation, biology, neurobiology, etc. The PDE theory on networks has been mainly applied to physics (stability of networks of strings, atomic reticular structure, propagation of electrical signal, etc) and to some simple models in neurobiology. But the recent interest in complex systems is bringing to the forefront more and more new applications of differential equations on networks which can not be embedded in a standard framework.

In turn, new fields are opened to mathematical investigation by the study of problem on networks: for example, over the last ten years, the study of traffic flow problems has pushed forward the analysis of conservation laws and fluid-dynamical systems on networks.

The research aims to develop some new techniques applicable to PDE arising as models of biological processes which share the following features:

- the problem models a biological process evolving on an irregular geometric structure (network, ramified space or fractal);
- the interactions among the components take place through interfaces which show some active behavior and can be controlled by an external agent.

For the different models considered, we analyse the following theoretical aspects:

- Well-posedness of the mathematical formulation of the problem
- Asymptotic problems: long time behavior, stability and ergodicity, pattern formation
- Numerical methods

Examples of problems considered by this research group are:

### **Chemotaxis on networks:**

The Keller-Segel model for chemotaxis is a celebrated model introduced in the 1970s in botany to study the aggregation of slime mold amoebae. In the course of the years it has become a general paradigm to describe the movement of organisms or cells according to the distribution of a chemical substance and a huge quantity of papers has been written about the mathematical, biological and medical aspects of chemotaxis. In some applications it is interesting to study this model on network: the plasmodium of the slime mold *Physarum polycephalum* contains a network of tube which enables nutrients and chemical signals to circulate through the body. It has been observed that in the search of food resources, the plasmodium is able to find the shortest routes in complicated networks and mazes [2]. In our research, we give an appropriate definition of the Keller-Segel model on the networks and we show its well-posedness. Moreover we explain via an asymptotic analysis the path-finding behaviour of amoeboid organisms observed by biologists.

### **Mean Field Games on networks:**

Mean Field games (MFGs) are models for large populations of interacting rational agents. These games are determined by a system of partial differential equations that comprises a Hamilton-Jacobi-Bellman equation coupled with a Fokker-Planck equation. MFGs were developed having in mind applications such as price formation, study of non-renewable resources, crowd motion, consensus formation, etc. MFGs on networks are motivated by the modeling and performance analysis of active networks for Internet access and traffic models. To extend the MFG theory to networks, we developed a suitable theory finding appropriate transition conditions to impose at the vertices of the network. Furthermore, we studied numerical methods for these problems to validate the choice of different MFG models.

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## M-4. Fractional and anomalous diffusions on fractals

*R. Capitanelli, M. D'Ovidio*

In recent years, there has been an increasing interest in studying stochastic processes and the corresponding operators on fractals. We notice that the path of a given particle can be regarded as a realization of a well specified stochastic process. From a physical point of view, such a study is justified by the fractal structure of the nature, to wit an increasing number of natural phenomena do not fit into the simple description of diffusion, developed for instance, by Einstein (or Smoluchowski and Bachelier). That is, "Nature is not standard". For example, the celebrated Brownian motion has been introduced as an erratic motion of pollens of *Clarkia* and described by Einstein giving rise to an important branch of modern Mathematics. Anyway, Brownian motion represents an ideal diffusion on homogeneous media. In nature, the medium in which a particle moves is non-homogeneous and the models usually considered refer to anomalous diffusions: a particle can find regions in which it spreads faster or slower than in other regions. In this case, we are able to find a suitable stochastic model by considering a time changed Brownian motion where the new clock changes randomly the velocity of the Brownian particle. A more detailed approach is based on the geometric characterization of the medium. Indeed, we can consider a medium with a fractal structure and the particle moves on it as a so called fractional diffusion. Fractals have been widely used as models of irregular media in which a lot of physical effects occur, like electrostatic charge distribution, heat diffusion, wave propagation and so on. Thus, we say that a diffusion, that is the movement of a particle, is anomalous and/or fractional meaning that the medium in which the particle is moving can have different space structures (fractal for instance). This leads to an anomalous behaviour of the particle inside the domain. Particular attention must be also paid on the particle behaviour near the boundary of the domain. In our case, the particle reflects inside not in the same way in every point of the boundary. A special example could be a semi-permeable membrane. The problems we are interested in are therefore well-described by fractional and anomalous diffusions in bounded domains and reflecting on the boundaries. In particular, our attention is directed towards irregular domains and our models describe irregular diffusions. Moreover, the reflections take place on irregular boundaries. A number of physical, biological, chemical and industrial processes are based on this dynamics. Indeed, such models turn out to be useful to describe 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 focus on the following directions of research:

I) provide mathematical tools describing the fractional and/or anomalous diffusions in confining media introduced above;

II) provide a probabilistic treatment of the processes.

A key tool in the probabilistic approach of our analysis is the time change of stochastic processes. We describe an anomalous diffusion by means of a suitable time change of diffusion process, for instance Brownian motion. The diffusion we are dealing with is confined in a bounded domain and reflects on the boundary. The PDE's connections (that is the relationship between stochastic process and its governing partial differential equation) is given by the theory of pseudo-differential operators related to subordinate semigroups if the time change is given by a subordinator. Otherwise, we deal with time changed processes which can be either Markovian or not, according to the time change. We treat separately such cases. The non Markov process can be for example a sub-diffusion and the governing equation involves a (Caputo) fractional derivative in time. We have to study the properties of the time-change which is, in the case of Caputo derivative, the inverse to a stable subordinator.

It is worth to mention also that, by means of such a class of processes, we obtain an ensemble of models for phenomena with memory. If the time changed process is Markovian, we are in need of an additive functional increasing when the diffusion hits the boundary. The inverse to such a functional gives the time at which the diffusion is on the boundary. In such a way, we are able to characterize anomalous diffusions, that is irregular motions inside Euclidean domains. Moreover, our analysis is concerned with the characterization of a diffusion in presence of some interface conditions (for instance, the elastic or skew conditions corresponding to some semi-permeable membranes).

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## M-5. Fractional Derivatives and non linear dynamics

*M. D'Ovidio, P. Loreti*

Our aim was to model phenomena where the associated dynamics is well described by fractional equations (FE) and non linear equations (NE).

The fractional equations we are dealing with arise from applications of a large class of phenomena, namely population dynamics, cell growth, bacterial motion, smart materials, bird flight, pedestrian motion. A problem we approach is concerned with the fractional growth of populations and therefore, with the number of interacting particles which grows according to a non-linear fractional dynamic given by the logistic model. Fractional diffusions are driven by governing equations with fractional operators in time as the well-known Caputo derivative. Recently, new fractional operators in time have been considered: such operators are obtained by convolution and characterized by a general class of kernels associated to Bernstein functions. The pseudo-differential symbol of the fractional operator has a Bernstein representation given in terms of Levy measure. Thus, from a probabilistic view-point, the theory of fractional calculus we consider here, well accords with the theory of the time-changes for Markov processes. The study of innovative materials such as polymers (it is well-known that textile, petroleum and pharmaceutical industries have strong interests in the investigation of smart materials) brings about to challenging mathematical questions. These are related with solutions to Integro-differential equations and Mittag-Leffler functions. The mathematical studies of this class of equations need advanced notions of fractional calculus. Here, our aim is to consider a general operator in time and therefore a class of kernels for the integro-differential equations.

The solutions to fractional diffusion equations can be written in terms of new processes realized through time change. In particular, given a Markov process  $X$  driven by a Cauchy problem we are able to study the Cauchy problem with a fractional power of the operator acting on space (the fractional Laplacian for instance) by considering a subordination of  $X$  (a Markovian random time) whereas, we are able to study the fractional Cauchy problem (with fractional derivative in time) by considering a time change for  $X$  (a non Markovian random time, the inverse to a subordinator). Since a Levy measure characterizes uniquely a subordinator (a non-negative increasing Levy process) we can associate to each fractional operator only one inverse to a subordinator (that is an hitting time for a subordinator). The mathematical approach is based on the changed semigroups and is related with the Bochner integrals. We remark that, also starting from a Markov process, the time changed process is not Markovian.

The well-known Verhulst model has been a prototype for many other studies and also the basic equation for

the study of more complicated processes. Its fractional logistic equation has been discussed in several contexts, we started from this equation and found the explicit representation of the solution. Our further investigation in the field of non linear equations has included also the study of the porous medium equation and the connection with the probabilistic theory. Fractional equations have been considered so far in order to study, macroscopically, the so called anomalous diffusions. In this contest, slow and fast diffusions driven by the porous medium equation have been often associated to anomalous diffusions. Macroscopically, they have been described by fractional diffusion equations.

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## M-6. Anzellotti's pairing theory and applications

V. De Cicco, D. Giachetti, F. Oliva, F. Petitta

In a 1983 pioneering paper, Anzellotti established a pairing between a divergence-measure vector field  $A$  and a function  $u$  of bounded variation, which is a suitable generalization of the scalar product between  $A$  and the measure gradient  $Du$ .

In some recent papers we generalized this pairing and introduced a nonlinear version of the notion of Anzellotti's, motivated by possible applications to evolutionary quasilinear problems. As a consequence of our analysis, we proved a generalized Gauss–Green formula, which extends the formula proven by De Giorgi in the sets of finite perimeter. This unifying result is obtained by revisiting the Anzellotti's pairing theory and by studying the singular part of the measure pairing. These results are contained in the papers [7] and [8].

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. We mention many papers of Chen, Frid, Panov for applications in the theory of hyperbolic systems of conservation and balance laws. Moreover we cite a paper of Ambrosio, Crippa and Maniglia for the case of vector fields induced by functions of bounded deformation, with the aim of extending the Ambrosio–DiPerna–Lions theory of the transport equations. Our contribution in this framework are contained in the papers [1], [3] and [6].

Another field of application is related to the Dirichlet problem for equations involving the 1–Laplacian operator. The interest in this setting comes out from an optimal design problem in the theory of torsion and from the level set formulation of the Inverse Mean Curvature Flow. On the other hand, it also appears in the variational approach to image restoration. Indeed, total variation minimizing models have become one of the most popular and successful methodology for image restoration since the introduction of the ROF model by Rudin, Osher and Fatemi. In this paper a variational problem involving the total variation operator is considered. It was designed with the explicit goal of preserving sharp discontinuities (edges) in images while removing noise and other unwanted fine scale detail. The 1–Laplacian operator emerges through the subdifferential of the total variation. Since that paper, there has been a burst in the application of the total variation regularization to many different image processing problems which include inpainting, blind deconvolution or multichannel image segmentation. To deal with the 1–Laplacian  $\Delta_1 u := \operatorname{Div} \left( \frac{Du}{|Du|} \right)$ , the main difficulty is to define the quotient  $\frac{Du}{|Du|}$ , being  $Du$  a Radon measure. This difficulty has been overcome

by Andreu, Ballester, Caselles and Mazón through the Anzellotti's theory of pairings. Namely, the role of this quotient is played by a vector field  $A$  having measure divergence such that  $\|A\|_\infty \leq 1$  and  $(A, Du) = |Du|$ . We studied some problems involving the 1-Laplace operator in [9] and [10].

Finally, in some lower semicontinuity problems for integral functionals defined in Sobolev spaces and in  $BV$ , the vector fields with measure–derivative occurred as natural dependence of the integrand with respect to the spatial variable. The lower semicontinuity of integral functionals is the starting point in order to establish the existence of minimum problems by using the direct methods of the Calculus of Variations. In recent years there has been a renewed interest in these topics since the lower semicontinuity in  $BV$  is used in a different way by many authors in new contexts, for instance in order to study some generalization of the Euler equation. For lower semicontinuity problems in  $BV$  see [2], [4] and [5].

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## M-7. Homogenization for singular semilinear elliptic problems

*D. Giachetti*

Some physical phenomena lead to mathematical models governed by semilinear elliptic equations with singular lower order terms whose simplest example is

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

where  $\gamma > 0$ , and  $f$  is nonnegative. Some of these physical situations deal, for example, with non newtonian pseudoplastic fluids or with diffusion in electrical conductors.

Of course, this kind of phenomena can take place in materials which are finely mixed according to a positive parameter  $\epsilon$  like, for example, metamaterials which are composite materials that "gain their properties from their structure, besides their composition; their precise shape, geometry, size, orientation and arrangement can affect the waves of light or sound in an unconventional manner, creating material properties which are unachievable with conventional materials." ([1])

In this case we are led to study the asymptotic behaviour, as  $\epsilon$  goes to zero, of a sequence  $(P_\epsilon)$  of semilinear singular problems. This process which starts from a microscopic description of the problem and provides at the end a macroscopic, or effective, description of the problem is called homogenization.

Let us describe two of these situations.

The first situation deals with (existence and) homogenization for elliptic problems with lower order terms singular in the  $u$ -variable ( $u$  is the solution) in a cylinder  $Q$  in  $R^N$ , so that the lower order term becomes infinite on the set  $\{u = 0\}$ . A rapidly oscillating interface  $\Gamma_\epsilon$  inside  $Q$  separates the cylinder in two composite connected components  $Q_{\epsilon 1}$  and  $Q_{\epsilon 2}$ . The interface has a periodic microstructure and it is situated in a small neighbourhood of a hyperplane which separates the two components of  $Q$ . At the interface we suppose the following transmission conditions: (i) the flux is continuous, (ii) the jump of a solution at the interface is proportional to the flux through the interface. This is a steady state model for the heat conduction in two heterogeneous electrically conducting materials with an imperfect contact between them. Our model is the following

$$\begin{cases} -\operatorname{div}(A^\epsilon \nabla u_\epsilon) = f \zeta(u_\epsilon) & \text{in } Q_{\epsilon 1} \cup Q_{\epsilon 2}, \\ [A^\epsilon \nabla u_\epsilon] \cdot \nu_\epsilon = 0 & \text{on } \Gamma_\epsilon, \\ (A^\epsilon \nabla u_\epsilon)_1 \cdot \nu_\epsilon = -\epsilon^\gamma h^\epsilon[u_\epsilon], & \text{on } \Gamma_\epsilon, \\ u_\epsilon = 0 & \text{on } \partial Q, \end{cases}$$

where  $A^\epsilon(x) = A(x/\epsilon)$  with  $A$  bounded uniformly elliptic periodic matrix,  $\zeta(s)$  is a nonnegative real function

singular at  $s = 0$ ,  $f$  is a nonnegative datum (not identically zero) whose summability depends on the growth  $\theta$  of the singular function  $\zeta(s)$  near the singularity  $s = 0$  and  $\nu_\epsilon$  is the unit outward normal to  $Q_{\epsilon 1}$ .  $[\cdot]$  denotes the jump through  $\Gamma_\epsilon$ . In [3] we prove that the different behaviour of the limit problem depends on the parameter  $\kappa$  which measures the amplitude of the oscillation of the interface and on the parameter  $\gamma$  (which appears in the proportionality coefficient between the flux and the jump of the solution through the interface).

The second situation concerns (existence, uniqueness, stability and) asymptotic behaviour, as  $\epsilon$  goes to zero, of a sequence of singular semilinear problems posed in domains  $\Omega^\epsilon$  obtained by removing many small holes from a fixed domain  $\Omega$ , in the spirit of [2]. The problem looks like

$$\begin{cases} -\operatorname{div} A(x) Du^\epsilon = f \zeta(u_\epsilon) & \text{in } \Omega^\epsilon, \\ u^\epsilon = 0 & \text{on } \partial\Omega^\epsilon. \end{cases}$$

The general questions we are concerned with are the following. Do the solutions  $u^\epsilon$  converge to a limit  $u$  when the parameter  $\epsilon$  tends to zero? If this limit exists, can it be characterized? Will the result be the same result as in the non singular case? In principle the answer is not obvious at all since, as  $\epsilon$  tends to zero, the number of holes becomes greater and greater and the singular set for the right-hand side (which includes at least the holes' boundary) tends to "invade" the entire  $\Omega$ .

Actually in [4] and [5] we prove that a strange term  $\mu u$  appears in the limit of the singular problems in the same way as in the non singular case studied in [2]. This result is a priori not obvious at all, and a very different behaviour could have been expected.

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## M-8. Interfaces and scaling laws in nonlinear PDEs

L. Giacomelli, F. Petitta

This research line focuses on carefully selected classes of nonlinear Partial Differential Equations (PDEs) in which the evolution of free boundaries, interfaces, and/or singularities plays a crucial role. 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 asymptotic and scaling laws. This requires a blend of tools from both the applied math community such as numerical simulations and matched asymptotic expansions and the PDE one such as integral estimates and variational techniques. Some selected results obtained within this framework between 2015 and 2017 are outlined below.

### Wetting phenomena and the thin-film equation.

The height of a droplet spreading over a substrate is typically described by the *thin-film equation*, which in non-dimensional variables reads as

$$\partial_t h + \nabla \cdot ((h^3 + b^{3-n} h^n) \nabla \Delta h) = 0 \quad \text{on } \{h > 0\},$$

with  $n \in (0, 3]$  and  $b > 0$  accounting for liquid-substrate frictional forces. In the *complete wetting* regime –which

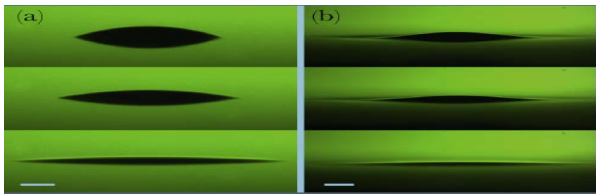


Figure 1: Silicone oil droplets spreading on thin films of the same oil with different thicknesses [PRL 109 154501 (2012)].

also models moist or pre-wetted substrates, see Fig.1– various formal asymptotics predicted the “macroscopic” droplet’s profile,  $h > b$ , to depend only logarithmically on the “microscopic” parameter  $b \ll 1$  at intermediate time-scales. In [1], through a detailed analysis of traveling-wave solutions, we have given rigorous bases to these asymptotics, setting the correct length-scale in the logarithmic dependence and showing that the mobility exponent  $n$  has no leading-order effect on the droplet’s macroscopic properties.

**Size effects in plasticity theory.** At micron scales, the behavior of metals displays a strong size-dependence, with smaller samples having higher relative strength and hardness (i.e., triggering plastic flow and attaining the same displacement require relatively more work). An evidence of size-dependent hardness is reported in Fig.2. With the aim of modeling these effects, several *gradient-plasticity* theories have been developed, most of them augmenting conventional plasticity with either “energetic” or “dissipative” length-scales. In [2], we have analyzed one of the best known among them (see Gurtin et

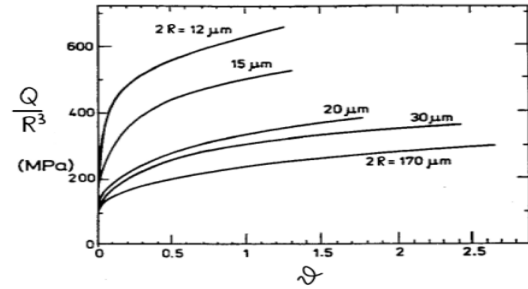


Figure 2: Torsional response of copper wires: the same normalized torque  $Q/R^3$  produces a smaller twist  $\vartheta$  on wires of smaller radius  $R$  [Acta Metall. Mater. 42 475 (1994)].

al., Cambridge University Press, 2010) in simple shear symmetry: via a combination of variational, PDE, and asymptotic arguments, we have rigorously confirmed that the model captures the experimental evidence that “smaller is stronger”, quantifying such scale effects.

**Flux-saturated diffusion equations.** Flux-saturated diffusion equations are second-order parabolic equations which, generally speaking, have the form

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

( $m \geq 0$ ). In essence, the flux  $\mathbf{j}$  remains bounded as  $|\nabla u|$  becomes unbounded. They find application whenever a saturation mechanism at high gradients, imposing a priori bounds on speed or flux, is modeling-wise relevant. In the “large gradient” regime, flux-saturated equations display a hyperbolic scaling, thus sharing many features with nonlinear conservation laws. Indeed, in [3,4] we have shown that the solution’s support expands with finite speed and that waiting-time phenomena may occur –i.e., a positive time may exist during which the support does not expand. Optimal bounds in terms of time-scales have been found for both phenomena.

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<http://www.sbai.uniroma1.it/~lorenzo.giacomelli/research.html>

## M-9. Fast diffusion across fractal interfaces

*M.R. Lancia*

It is by now well established that in many natural and industrial processes diffusion phenomena take place across disordered and wild media. We mention here only some examples, such as the diffusion of sprays in the lungs, the current flow across rough electrodes in electrochemistry and the diffusion processes in physiological membranes. In these contexts irregular interfaces of fractal type are of great interest, since many irregular media are believed to exhibit fractal properties.

Fractal interfaces, in general, can provide a useful tool in all those models in which one wants to enhance the absorption effects of the layer by increasing its surface, that is, in all those problems with large surfaces confined in small volumes.

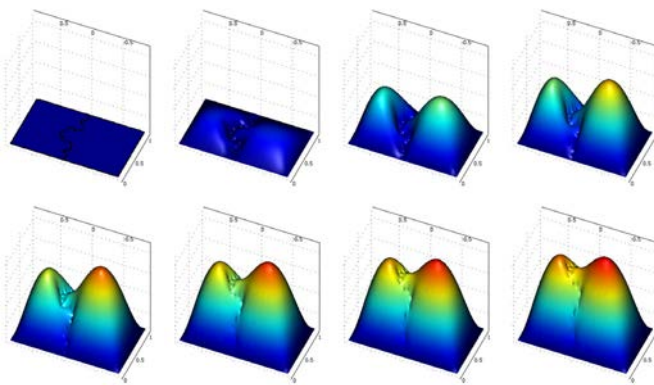


Figure 1: Heat flow across a Koch-type prefractal interface

Fractals are irregular geometric objects that display self-similarity. Self-similar objects have the property to be composed, on every scale, of parts that are similar to the structure of the overall object. Many anatomic structures display fractal-like geometry, for example, arterial and venous trees, the branching of certain cardiac muscle bundles or tracheobronchial trees.

Our research has been focusing on some fast-diffusion phenomena across irregular boundaries of fractal type, which are modeled by the so-called *Venttsel' problem*:

$$\begin{cases} \frac{du}{dt} - \mathcal{L}[u] = f & \text{in } \Omega, \\ \frac{du}{dt} + \frac{\partial u}{\partial \nu_{\mathcal{L}}} - \mathcal{L}_{\partial\Omega}[u] + bu + \theta(u) = g & \text{on } \partial\Omega, \\ u(0, x) = u_0(x) & \text{in } \bar{\Omega}, \end{cases}$$

where  $\mathcal{L}$  is a general differential operator of order  $p \geq 2$ , which can be also of non-divergence type,  $\Theta$  is a non local operator.  $\Omega$  is a two or three dimensional domain with fractal boundary or interfaces

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. Since our aim was to consider the corresponding numerical approximation, we considered also the corresponding problems in the so-called prefractal (smoother) domains. We proved that the approximating prefractal solutions do converge, in a suitable sense, to the limit fractal one, see [1,2,3,4]. As an application we studied heat propagation problems across an infinitely thin highly conductive layer of prefractal type both from a theoretical and a numerical point of view see figure 1.

The numerical approximation of evolution problems across irregular layers is also recent. In previous papers we have developed efficient algorithms capable to generate mesh for domains with fractal boundaries or interfaces.

From the point of view of applications our results may allow for the development of new generation of optimal cooling systems for electronic devices, solar panels, catalytic converters and the more challenging frontiers of nanostructural hydrophobic surfaces. It is to be pointed out that our results pave the way to another complete different fields of application, they can be regarded as a first preliminary step towards the study of the evolution of dendritic interfaces. Dendrites are organic cells characterized by branches which extend from the center of the cell in various directions. For instance, some cells of the human body are dendrites. The goal of our research is to model by fractal interfaces the diffusion across and along dendrites.

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## M-10. Singular elliptic Dirichlet problems

*F. Petitta, D. Giachetti, F. Oliva*

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

$$\begin{cases} -\Delta u = \frac{f}{u^\gamma} & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \quad (\text{P}_\gamma)$$

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

Physical motivations in the study of problems as  $(\text{P}_\gamma)$  arise, for instance, in the study of thermo-conductivity where  $u^\gamma$  represents the resistivity of the material, in signal transmissions, and in the theory of non-Newtonian pseudoplastic fluids. Equations as in  $(\text{P}_\gamma)$  also appear as a model of boundary layers.

From the purely mathematical point of view, a systematic treatment of problems as  $(\text{P}_\gamma)$  was developed starting from the 70's by many contributors as W. Fulks, J. S. Maybee, C. A. Stuart, M. G. Crandall, P. H. Rabinowitz and L. Tartar.

If  $f$  is smooth enough (say Hölder continuous) and bounded away from zero on  $\Omega$  then the existence and uniqueness of a classical solution to  $(\text{P}_\gamma)$  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 by A. C. Lazer, P. J. McKenna in 1991 by proving, in particular, that  $u \notin C^1(\bar{\Omega})$  if  $\gamma > 1$  and it has finite energy, i.e.  $u \in H_0^1(\Omega)$ , if and only if  $\gamma < 3$ .

Classical theory for equations as in  $(\text{P}_\gamma)$ , also called singular Lane–Emden–Fowler equations, has been also extended to the case in which the term  $s^{-\gamma}$  is replaced by a  $C^1$  nonincreasing nonlinearity  $h(s)$  that blows up at zero at a given rate.

More general situations can be considered. Let  $f$  be a nonnegative function belonging to some  $L^m(\Omega)$ ,  $m \geq 1$ , or even, possibly, a measure. If  $f \in L^1(\Omega)$ , L. Boccardo and L. Orsina recently proved the existence of a distributional solution  $u$  to  $(\text{P}_\gamma)$ .

In the case of  $f$  being a measure the situation becomes striking different. Nonexistence of solutions to problem  $(\text{P}_\gamma)$  is proven (at least in the sense of approximating sequences) if the measure is too concentrated, and sharp existence results are obtained if the measure is diffuse; here concentration and diffusion is intended in the sense of capacity (see [2]).

Consider now the boundary-value problem

$$\begin{cases} Lu = h(u)f + \mu & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \quad (\text{P}_h)$$

where  $L$  is a linear elliptic operator in divergence form,  $h: \mathbb{R}^+ \rightarrow \mathbb{R}^+$  is a continuous function that may blow up

at  $s = 0$  and possesses a limit at infinity,  $f$  and  $\mu$  are nonnegative functions in  $L^1(\Omega)$  (or, possibly, bounded Radon measures on  $\Omega$ ).

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  $\mu \equiv 0$  and  $f$  is only a nonnegative function, then the solutions do not belong in general to  $H_0^1(\Omega)$  even for small  $\gamma$  nor the lower order term in  $(\text{P}_h)$  needs to belong to  $L^1(\Omega)$ .

In particular, the question of the summability properties of the lower order term in  $(\text{P}_h)$  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  $(\text{P}_\gamma)$ .

General existence, uniqueness and regularity results for solutions to  $(\text{P}_h)$  have been studied both in the model case  $h(s) = s^{-\gamma}$  ([1]) and in the case of a suitably summable function  $\mu$  ([3]).

If  $\mu \equiv 0$ , in [4], under fairly general assumptions a natural notion of distributional solution to problem  $(\text{P}_h)$  can be introduced for which existence can be shown to hold. Moreover, uniqueness holds provided  $h$  is nonincreasing. As we already mentioned, particular care has to be addressed on how the homogeneous boundary datum for the solution  $u$  is (weakly) attained.

If  $f$  is a function in  $L^m(\Omega)$ ,  $m \geq 1$ , one may also investigate the question of whether the solution to problem  $(\text{P}_h)$  has finite energy eventually yielding well posedness in  $H_0^1(\Omega)$ . One can 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. Additionally, one obtains sharp thresholds for the lower order term to belong to  $L^1(\Omega)$ . The results and their optimality can be shown through appropriate examples.

Also hinted by the previously mentioned examples, in the general case of a measure as datum, a key tool in order to prove uniqueness is the establishment of a weighted summability estimate on the lower order term  $h(u)f$ . Then uniqueness of a solution is obtained by mean of a suitable Kato type inequality.

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## M-11. Numerical Solution of Fractional Differential Equations

L. Pezza, F. Pitolli

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 (as in Unser and Blu) 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], nonlinear fractional differential problems [4,5] and diffusion problems having time derivative of fractional order [6,7].

As an exemple, we consider the *time-fractional differential diffusion problem*

$$\begin{cases} D_t^\gamma u(t, x) - \frac{\partial^2}{\partial x^2} u(t, x) = f(t, x), t \in [0, T], x \in [0, 1], \\ u(0, x) = 0, x \in [0, 1], \\ u(t, 0) = u(t, 1) = 0, t \in [0, T], \end{cases} \quad (1)$$

where  $D_t^\gamma u$ ,  $0 < \gamma < 1$ , denotes the *Caputo partial fractional derivative* with respect to the time  $t$  defined as

$$D_t^\gamma u(t, x) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{u_t(\tau, x)}{(t-\tau)^\gamma} d\tau, \quad t \geq 0, \quad (2)$$

Here,  $\Gamma$  denotes the Euler's gamma function.

The *fractional spline collocation-Galerkin method* we proposed [6] combines the fractional spline collocation method introduced in [2] for the time discretization and a classical spline Galerkin method in space. The method is proved to be convergent. Moreover, the numerical tests show that the method is efficient and accurate.

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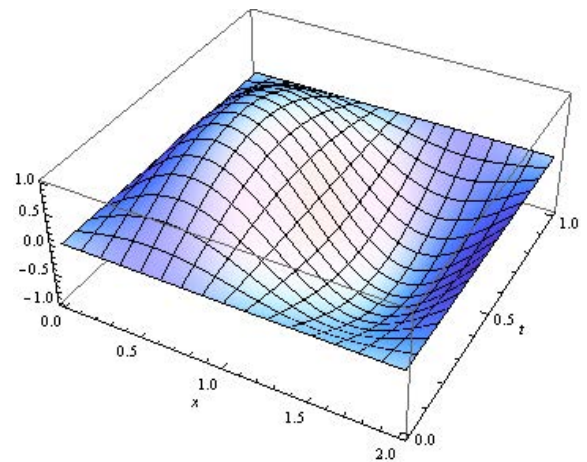


Figure 1: The numerical solution for  $\gamma = 0.25$  and  $\Delta t = \Delta x = 0.03125$ .

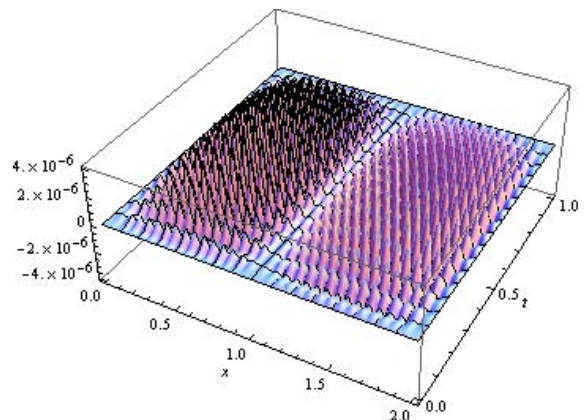


Figure 2: The error for  $\gamma = 0.25$  and  $\Delta t = \Delta x = 0.03125$ .

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## M-12. Decision models under ambiguity

*B. Vantaggi*

Probability and statistics have been the only well-founded theories of uncertainty for a long time.

However, during the last fifty years, in some areas like decision theory, economic theory, artificial intelligence and information processing, numerous approaches generalizing or departing from the existing theory of probability and mathematical statistics have been successfully developed. Thus, new inputs have been given also to the classical theories.

The common feature of all those attempts is to allow for a more flexible modelling of uncertainty, imprecision, vagueness.

The proposed new methods are softer than the traditional theories and techniques because, being less rigid, they adapt to the actual nature of information in a more natural way.

In many problems of choice under uncertainty, the available information is often far from being sufficiently precise to allow the decision maker to come up with an estimate of a probability distribution over the relevant states of nature.

The archetypical example of such a situation is the Ellsberg paradox, in which subjects have some imprecise information concerning the composition of an urn: the probability of drawing a red ball from the urn is one-third whereas the probability of drawing a yellow ball is anything between zero and two-thirds. Under such conditions, the decision maker is faced with a bet that depends on the outcome of the experiment and he/she needs to consider the possible compositions of the urn that generate a class of probability measures.

The usual finding in this experiment is that preferences of subjects cannot be represented by an expected utility functional, computed with respect to a single probability measure, rather, one should assume that subjects have “multiple beliefs”. Ellsberg paradox can be managed under a subjective set of priors by computing the worst expected value of a gamble over this set of selected priors.

Ambiguity refers to those situations where the available information does not allow to single out a single probability measure, but a class of probabilities must be considered instead.

This situation occurs, for example, when a statistical model is not identifiable as well as latent or hidden variables are present.

Ambiguity arises also when the observed variable could be a misclassified version of the variable of interest, and the misclassification distribution is not known. Inferential problems caused by data errors need to be studied by taking into account of the class of probability measures belonging to not identifiable regions. A method for estimating the identification regions is pro-

vided in [1], in the general case and under some specific restrictions on the misclassification mechanism. The method is illustrated with an empirical analysis arising from data involving Health and Administrative studies collected from different institutes, Italian National Institute of Statistics and the Centre for Economic and International Studies of University Tor Vergata.

Moreover, in dynamic environments, agents need to update their expectations upon the arrival of new information. This requires the introduction of a suitable updating rule for non-additive measures or for classes of probabilities. The adopted notion of conditioning is crucial in drawing inferences as it affects the final result of inferential processes.

For that a study of an updating rule is carried on for particular classes of probabilities and their envelopes. In [2] the classes having lower envelopes, which are infinitely monotone capacities, have been studied. While in [3] an updating rule has been investigated for the classes of probabilities giving rise to upper envelopes which are idempotent probabilities (maxitive measures).

The infinite monotone measures are induced, for example, by a finitely additive probability measure and multivalued map. In turn, a multivalued mapping can be considered as an imprecise random quantity used to transport probabilistic information from one space to another: this kind of maps are used in economics and statistics for handling partially identified models.

The inferential problems related to the transport of probabilistic information has been studied in [4], dealing also with the problem of conditioning to unexpected events, i.e., those of zero probability. In game theory and dynamic programming it is natural to consider finitely additive conditional probability, moreover, the possibility of updating the information with respect to events of zero probability reveals to be crucial as it deeply impacts on the analysis of a game.

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## M-13. Boundary value problems in irregular structures

*M.A. Vivaldi, F. Camilli, R. Capitanelli, S. Fragapane*

Our research mainly deals with theoretical and numerical aspects for quasi-linear problems in irregular structures. By irregular structures we mean fractals as well as domains with fractal boundaries. We point out some topics.

I) We have studied quasi-linear problems domains with fractal boundaries. In particular we have established regularity results for the solutions of obstacle problems involving  $p$ -Laplacian type operators on Koch Islands and on the polygonal domains approximating the Koch Islands in terms of the weighted Sobolev spaces and fractional Sobolev space. In case  $p > 2$ , to our knowledge, there are no regularity results in fractional Sobolev space with smoothness exponent greater than one for domains with fractal boundary. Our results concern obstacle problems in the approximating polygonal domains (see [1]).

II) We have also studied the asymptotic behavior of solutions of obstacle problems involving  $p$ -Laplacians on Koch Islands and on the polygonal domains approximating the Koch Islands Koch when  $p$  tends to infinity. In particular, we have proved that the solutions converge to a Monge-Kantorovich's potential for the mass transport problem, as in the case of regular domains (see [2]).

III) We have also faced the numerical approximation of obstacle problems involving  $p$ -Laplacian type operators on polygonal domains approximating the Koch Islands. We have established error estimates for the FEM-solutions. The regularity properties of the solution play a crucial role in the error estimates. Hence we have used the regular results obtained (see point I) to improve existing estimates (see [3]).

IV) We have also studied the  $p$ -Laplacian and the infinity-Laplacian on the Sierpinski gasket, the variational convergence of discrete energies to "fractal" energies and the asymptotic behavior of energies when  $p$  tends to infinity. We note that the results obtained can be readily extended to a larger class of fractals (the class of post-critically finite fractals) (see [4])

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## M-14. Algebraic and combinatorial aspects of orthogonal polynomials, hyperbolic polynomials, finite fields

*S. Capparelli, V. Pepe, A. Vietri*

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 2015, 2016, 2017. Described below in particular is that part of the research concerned with algebraic and combinatorial aspects of orthogonal polynomials (Dyck paths, root powers, “rencontres”, derangements), hyperbolic polynomials, finite fields.

1. In previous research papers certain combinatorial properties of orthogonal polynomial sequences arising from special matrices were studied. In [1] we took up a systematic study of some properties of the sequence of moments arising from a generalization of the matrices studied there. We used a combinatorial interpretation of the action of the binomial transform on the sequence of moments of orthogonal polynomials arising from a tridiagonal matrix to obtain relations that tie together different well-known sequences of integers. We also obtained a recursive formula for the moments. The object of our study was also the set of Dyck paths. We introduced an equivalence relation on the set of Dyck paths, we computed the cardinality of the equivalence classes and used this information to give a combinatorial formula for the number of Dyck and Motzkin paths of a fixed length.
  2. In [2] the 2-spreads of  $PG(5, q^2)$ ,  $q$  even, with some extra properties was studied. It was shown that  $S$  is a symplectic semifield spread of  $PG(5, q^2)$ ,  $q$  even and  $q \geq 2^{14}$ , whose associated semifield has center containing  $GF(q)$ , then  $S$  is Desarguesian.
  3. 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.
  4. 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.
- Other authors have confirmed these results and exhibited three polynomials of the desired type of degree 18. We decided to choose Chebyshev polynomials as a basis. When expressed in terms of Chebyshev polynomials often the desired polynomials appear to have coefficients with small absolute value and with a certain regularity. With this method, one of the three polynomials of degree 18 could have been found. Recently, A. Vietri is studying this problem and was able to reobtain several interesting polynomials. We determine certain conditions on the Chebyshev coefficient that guarantee that the given polynomial has roots in the interval  $[-2, 2]$ . We also study a certain generalization of roots of unity given by Salem numbers. We find certain families of polynomials that are essentially minimal polynomials of Salem numbers. To show this we use the classic construction of Salem starting from Pisot numbers. This will appear in a future paper.
5. 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  $X \cup U$ .

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## M-15. Geometric Methods in Representation Theory of Finite Dimensional Algebras

*G. Cerulli Irelli*

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 called *quiver Grassmannians*. Roughly, the research concerns the following aspects:

- Quivers and their representations;
- Quiver Grassmannians;
- Abelian degenerations of Lie algebras;
- Fomin-Zelevinsky cluster algebras.

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. A quiver Grassmannian attached to  $M$  is

$$\text{Gr}_{\mathbf{e}}(M) = \{N \subseteq_A M \mid \dim N = \mathbf{e}\}$$

where  $\mathbf{e}$  is a  $Q_0$ -graded dimension. This is a projective variety and every projective variety can be realized in this way. Quiver Grassmannians were first studied by Schofield in 1990 to get general properties of quiver representations and find a way to compute Kac's canonical decomposition, which was a main research area at that time. The interest for quiver Grassmannians increased in the last ten years, when it was discovered that their Euler characteristic can be used to find generators of Fomin-Zelevinsky cluster algebras. More precisely, what matters is the Euler characteristic of *rigid* quiver representations. The famous positivity conjecture of Fomin and Zelevinsky (2001) states that such Euler characteristic is positive. The conjecture was solved by Nakajima in 2011 using monoidal categorification of cluster algebras. A survey of the subject appeared in

[1]. A part from the Euler characteristic, it is natural to study other geometric aspects, such as existence of cellular decomposition or properties of the cohomology ring. In this direction, we recently obtained the following striking result [2]:

**Theorem:** 1) The odd cohomology spaces of a quiver Grassmannian attached to a rigid quiver representation are zero and the cycle map is an isomorphism. 2) Every quiver Grassmannian of finite type admits a cellular decomposition. 3) Every quiver Grassmannian attached to an indecomposable representation of an affine quiver admits a cellular decomposition.

The theorem above is proved by combining standard techniques in complex algebraic geometry together with representation theory.

In 2010, in connection with abelian degenerations of Lie algebras, E. Feigin found a class of projective varieties called degenerate flag varieties. They are flat degenerations of flag varieties and share many properties with Schubert varieties. It was noticed in [3] that indeed degenerate flag varieties are Schubert varieties. This observation lead to an active area of research. In [3] we introduced other degenerations of flag varieties that we call linear degeneration of flag varieties. Some of their geometric aspects are object of current investigation.

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## M-16. Umbral Calculus

*B. Germano*

The term "Umbral" has been initially proposed by S. Roman and G.C. Rota to stress, in an (at the time) emerging field of operational calculus, the common practice of replacing a series of the type

$$\sum_{n=0}^{\infty} c_n \frac{x^n}{n!}$$

representing a certain function  $f(x)$  with the formal exponential series

$$\sum_{n=0}^{\infty} c^n \frac{x^n}{n!}$$

The "promotion" of the index  $n$  in  $c_n$  to the status of a power exponent of the operator, namely the umbral operator, is the essence of "umbral", since it is a kind of projection of one into the other. We adopt the same starting point, but our conception of umbral and of technicalities developed are different.

The authors prove, for example, that Bessel function are the umbral images of the Gaussian. Albeit an apparently sterile exercise, such a point of view offers a wealth of new perspectives either for the study of the properties of old and new special functions and for introduction of novel computational methods and differential operational calculus.

The method has opened new avenues to deal with rational, transcendental and higher order transcendental functions, by the use of the same operational forms. The technique had been formulated in general enough terms to be readily extended to the fractional calculus. The starting point of our theory is the use of the Borel transform methods to put the relevant mathematical foundation on rigorous grounds.

Our target is the search for a common thread between special functions, the relevant integral representation, the differential equations they satisfy and their group theoretical interpretation, by embedding all the previously quoted features within the same umbral formalism.

The procedure we envisage allows the straightforward derivation of (not previously known) integrals involving e.g. the combination of special functions or the Cauchy type partial differential equations (PDE) by means of new forms of solution of evolution operator, which are extended to fractional PDE. It is worth noting that our methods allow a new definition of fractional forms of Poisson distributions different from those given in processes involving fractional kinetics.

We underscore the versatility and the usefulness of the proposed procedure by presenting a large number of applications of the method in different fields of Mathematics and Physics.

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## M-17. Finite geometry and combinatorics

V. Pepe, S. Capparelli

The main topics of our research are related to the study of algebraic varieties over finite fields and their applications on extremal combinatorics.

Let  $\mathbb{P}^{n-1}(F_q)$  be the projective space of dimension  $n-1$  over the finite field of order  $q$   $F_q$ .

One of our main interests are the so called  $F_{q^t}$ -linear set of  $\mathbb{P}^{n-1}(F_q)$ , i.e., points of the projective space defined by a vector space over the subfield  $F_{q^t}$  of  $F_q$ . We stress out that such a set does not necessarily define a  $\mathbb{P}^{m-1}(F_{q^t})$ , but it can define a wide range of geometric configurations. They have been used to construct, among others, semifields, blocking sets and maximum rank distance codes.

An equivalent to define a linear set is the following: in  $\mathbb{P}^{nt-1}(F_q)$  let  $\mathcal{D}$  be a Desarguesian  $(t-1)$ -spread, i.e., a partition of the point set of  $\mathbb{P}^{nt-1}(F_q)$  in  $(t-1)$ -subspaces with automorphism group  $\cong \text{PGL}(n, F_{q^t}) \times \text{Gal}(F_{q^t}/F_q)$ ; a linear set is the subset of  $\mathcal{D}$  with non-empty intersection with a fixed subspace of  $\mathbb{P}^{nt-1}(F_q)$ . We proved that the Grassmann embedding of  $\mathcal{D}$  is a subvariety of the Segre variety  $\underbrace{\mathbb{P}^{n-1}(F_{q^t}) \times \mathbb{P}^{n-1}(F_{q^t}) \times \cdots \times \mathbb{P}^{n-1}(F_{q^t})}_{t \text{ times}}$

consisting of pure tensors of type  $u \times u^q \times \cdots \times u^{q^{t-1}}$ , namely  $\mathcal{V}_{nt}$ . In [3], we hence observed that the Grassmann embedding of linear set is the intersection of a Schubert variety with  $\mathcal{V}_{nt}$ , we investigated the properties of the resulting variety and how to use this representation to study the properties of the linear set.

As we have already mentioned, linear sets are also used to construct semifields, or rather semifield spreads of projective spaces. Spreads of  $\mathbb{P}^{2n-1}(F_q)$  in  $(n-1)$ -spaces give arise to translation planes of order  $q^n$  via the well known André-Bruck-Bose construction and then semifields spreads are the ones that give arise to translation planes coordinatized by a semifield. Also, if the spread elements are totally isotropic with respect a symplectic polarity, then the correspondent semifield is commutative. A standard way to get such a spread is by constructing maximum rank  $F_q$ -linear sets of the space of symmetric matrices of order  $n$  over  $F_{q^t}$  disjoint from the variety of the singular matrices, i.e., the  $(n-2)$ -secant of the Veronese variety. The case  $n=2$  has been extensively studied. In [2] and [4], we dealt we the case  $n=3$  and we classified maximum rank linear sets disjoint from the secant variety of the Veronese surface in even characteristic. We have proved the general and conclusive result that the only possible spread has associated plane coordinatized by a field, hence a commutative semifield with the relevant parameter must be a field in even characteristic.

One of the most classical and important problems in extremal combinatorics is the forbidden subgraph problem: for a given graph  $G$ , find the maximum number

of edges for a graph with  $n$  vertices that does not contain a subgraph isomorphic to  $G$ . That number is also called the Turán number of  $G$  and denoted by  $ex(G, n)$ . When the chromatic number of  $G$  is larger than 2, then  $ex(G, n)$  is known, while for bipartite graphs the problem is still open. For the complete bipartite graph  $K_{s,t}$ , we have a lower bound for  $ex(K_{s,t}, n)$  obtained with probabilistic methods and an upper bound due to Kővari, Sós and Turán, KST bound for short, conjectured to be sharp. N. Alon et al. proved that the KST bound is sharp for  $K_{s,t}$  with  $t > (s-1)!$ . Our project started a few years ago. Together with S. Ball we have studied the following kind of graphs: the vertices are the points of an affine space over  $F_q$  and the neighbors of a point  $P$  are the points of an algebraic variety  $\mathcal{V}_P$ . By the appropriate choice of  $\mathcal{V}_P$ , one can construct large graphs with no  $K_{s,t}$ . We obtained several results with this approach and in the period 2015-2017, in [1], we have constructed graphs with no  $K_{s,t}$  with  $t \geq (s-2)! - 1$  with a number of edges larger than the probabilistic lower bound, hence, at the moment, this is the best deterministic construction for  $K_{s,t}$  with  $(s-2)! - 1 \leq t \leq (s-1)!$ .

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## M-18. Graph colouring and graph labelling: some connections with geometry and algebra

A. Vietri

A *graph* is a collection of points (*vertices*) together with a collection of *edges* connecting some (or possibly all) pairs of vertices. In many applicative questions related to graphs it is important to *colour* the edges in such a way that adjacent edges be coloured differently. The least number of colours that are needed is a crucial information. *Critical graphs* with respect to edge-colouring are special graphs, in that the number of colours they require decreases if any edge is removed.

One of the projects in this report is centered around the construction of critical graphs by means of small patterns which are properly connected so as to form a global graph which is critical. The key property of these patterns is the capability of transmitting, deterministically, a certain colour from one end to the other, across the pattern. Vietri in [1] provided a new classification of small critical graphs of degree 3 as listed by I.T. Jacobsen. His approach relates topology to graph theory. A prototype in this regard is provided by any odd cycle. Such a graph needs at least 3 colours, but the number decays to 2 after a cut. This is actually the same behaviour (*mutatis mutandis*) as in the Möbius strip case: both the combinatorial and the geometrical entities under examination are the result of a suitable identification.

In collaboration with S. Bonvicini, Vietri has analysed the just larger degree, 4, by constructing new infinite families of critical graphs and revisiting classical examples such as (a) and (b) in Figure 1 (see [2]). Again, small patterns play a major role and the spirit of the paper is the same as above.

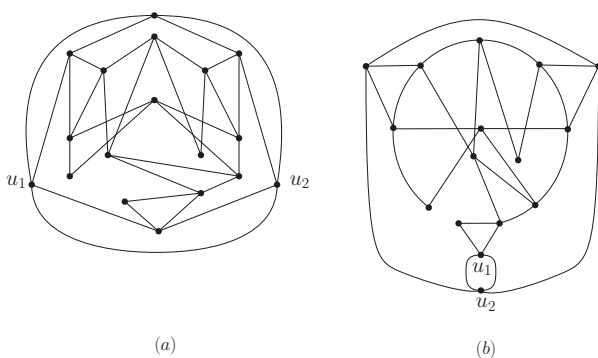


Figure 1: Fiol's and Chetwynd's critical graphs

Besides the reported geometric approach, an algebraic structure has been associated to graphs in order to analyse some properties related to vertex labellings. In [3] Vietri has associated a family of homogeneous polynomials (*graceful polynomials*) to a given graph, using as many variables as the number of vertices. Such polynomials are related to *graceful labellings* (see Figure 2):

a graceful polynomial with all even coefficients can be successful in proving that a graph is non-graceful. These polynomials have a rich structure and can therefore be analysed on their own right. The main result in [3] is the classification of graphs whose graceful polynomial has all even coefficients, for small degrees of the polynomials, up to 4.

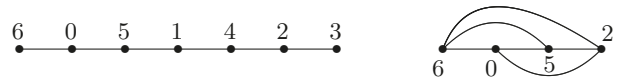


Figure 2: Graceful labellings for the 6-path and the complete graph  $K_4$

A different way of assigning labels to vertices is deeply related to group and ring theory. A *zero-divisor graph* connects all pairs of elements of a given ring whose product is the zero element. In [4] Vietri has classified all possible zero-divisor graphs of a particular family of quotients of  $\mathbf{Z}_4[x, y, w, z]$ . The novelty of this approach is that many distinct cases have been collected together by looking at the underlying combinatorial structure of the graph instead of the single properties of the ring elements. This has allowed for a faster check – with respect to the previously known techniques – of all possible configurations and a consequently easier management of the many cases. In a previous paper the graph-theoretical technique was first introduced by Vietri and it was applied to  $\mathbf{Z}_4[x, y, z]$  in order to study a classical counterexample related to zero-divisor graphs (see *Beck's conjecture*).

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## M-19. The world of $C^*$ -algebras: general aspects and applications to Quantum Field Theory

*R. Conti*

Research in the period 2015-2017 has mostly focused on the following topics.

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

The results of these studies have been collected in about 15 articles, among which at present 12 have been already published (or accepted for publication) and 3 are still under the referee process.

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 analysis of the structure of crossed products associated to  $C^*$ -dynamical systems, and especially it is concerned with uniform Fourier expansion, asymptotic invariance properties, (semigroups of) completely positive maps, etc.

The second item includes the study of several properties of the automorphism group and endomorphism semigroup of Cuntz-like algebras, with very challenging connections with the theory of semisimple Lie groups but also discrete mathematics and combinatorics.

The third item follows a new line of research initiated by V. Jones (Field Medalist 1990) and inspired by Topological 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 graph and knot/link invariants; coefficients of these representations might then be related to analytic and algebraic properties of these fascinating but complicated groups.

Roughly, noncommutative geometry is a replacement of differential geometry in the noncommutative setting. As abstract  $C^*$ -algebras describe noncommutative topological spaces, spectral triples then describe spaces with differential structures (e.g., connections, spin structure). The fourth item is about 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  $\lambda \rightarrow 0$ . After a general analysis, most of the subsequent work has been devoted to study a concrete but important example, namely the so-called Schwinger model in  $D = 1 + 1$ , for which some charges appear in the scaling limit that are not present at the ambient scale (confinement).

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.

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## M-20. Discrete harmonic analysis and representation theory

*F. Scarabotti*

Representation theory and harmonic analysis can be used to study problems with a large group of symmetries, in many areas of pure and applied mathematics. In particular, there are many combinatorial and probabilistic problems that may be translated into spectral problems and then solved by commutative or non commutative harmonic analysis. The discrete case is treated in our recent monograph [1].

Gelfand pairs constitute a powerful bridge between commutative and non commutative methods, because they arise from commutative subalgebras in non commutative convolution algebras. The associated spherical functions may be used to define very effective spherical Fourier transforms.

We have studied the Frobenius-Schur indicator theorem in the setting of  $\tau$ -conjugate representations of finite groups. We have developed a similar theory in the context of Gelfand pairs. Moreover, we have discussed a detailed version of the so-called Gelfand criterion for weakly symmetric Gelfand pairs and a characterization of simply reducible groups, a notion introduced by Wigner for applications to physical problems [2].

We have also obtained a useful criterion for multiplicity-freeness of the decomposition of the restriction to a subgroup  $H$  of the Kronecker product of two generic irreducible representations of a finite group  $G$ . We have illustrated the corresponding harmonic analysis by means of detailed computations on the Clifford group  $CL(n)$ , together with the subgroup  $CL(n-1)$  [3].

Observing that, in the setting of finite groups, a Gelfand pair may be seen as a multiplicity free representation obtained by inducing the trivial one, we have generalized all the machinery of spherical functions to the setting of any induced representation. We have included several detailed computations with the affine group over a finite field [4].

We are currently investigating several generalizations of Gelfand pairs defined by means of finite groups. In particular, we are developing harmonic analysis of multiplicity free induced representations with the construction of interesting example by means of finite linear groups.

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## M-21. Asymptotic behavior for nonlinear parabolic equations

*D. Andreucci*

Consider an initial value problem for a partial differential equation of parabolic type; that is, besides satisfying the differential equation in the prescribed domain, we require that the solution coincides at the initial time with a given function (the initial value). If the domain has a non-empty boundary we assume here that a null flux condition is prescribed (Neumann problem with zero data); for example this implies the property of conservation of mass which is of course relevant both from a mathematical and an applicative point of view, since the problems at hand are in general models of some diffusion process. We also assume in this connection that the solution is non-negative, which allows its identification with a density. In turn, this property follows usually from the maximum principle and the assumed non-negativity of the initial data.

A classical problem is the investigation of the asymptotic behavior of such solutions for large times, which is of importance in theory and application. If the initial data is integrable, i.e., the total mass is finite, and the domain has infinite volume, it is rather intuitive that the solution decays to zero as  $t \rightarrow +\infty$ . For example it is a classical result in this direction that solutions of the standard heat equation in the whole Euclidean space  $\mathbf{R}^N$  decay with a rate  $t^{-N/2}$ . A very interesting issue is the asymptotic profile approached in the limit by the solution; in the classical case just described all solutions approach in a suitable sense the profile of a fundamental solution with the correct mass, that is the solution to the initial-value problem with data given by a suitably scaled Dirac mass.

In the literature many contributions to this area are present. We summarize below our work in the period of interest. In general, we have aimed at generalizing the diffusion equation in order to admit nonlinearities and degeneracy, and the spatial domain to admit subdomains of the Euclidean space or Riemannian manifolds. However we keep the property of absence of sources or sinks in the equation, and only consider domains with infinite volume.

- In [1] we consider an equation of the so called doubly non-linear type, that is, in comparison with the linear case, we allow the diffusivity to depend both on the solution itself and on its gradient:

$$\frac{\partial u}{\partial t} - \operatorname{div}(u^{m-1} |\nabla u|^{p-2} \nabla u) = 0,$$

$m > 0$ ,  $p > 1$ ,  $m + p > 3$ . The domain is a Riemannian manifold without boundary and with infinite volume; its relevant metric properties are encoded in a Faber-Krahn inequality of suitable type, that is an inequality involving the integral norms of

compactly supported functions and of their gradients; the exact form of the inequality is expressed in terms of a function, called Faber-Krahn function, which enters all our main results. We prove sharp sup estimates both in the case of integrable initial data and of data growing at infinity, in a suitable sense.

The case just described would correspond in the Euclidean setting to the one of a domain expanding at infinity (say a paraboloid); we also look at the case where the Faber-Krahn inequality is valid only in every bounded subdomain of the manifold, which corresponds to domains narrowing at infinity (say an infinite cusp).

- In [2] we consider the equation

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x_j} \left( a_{ij}(x, t) \frac{\partial u^m}{\partial x_i} \right) = 0,$$

with  $m > 1$  in the paraboloid  $\Omega = \{x = (x', x_N) \in \mathbf{R}^N \mid |x'| < x_N^\alpha\}$ ,  $0 < \alpha < 1$ . Here the novelty is both in the allowed variability of the coefficients  $a_{ij}$  and in the shape of the domain. We prove that solutions with finite mass assume the asymptotic profile of a fundamental solution to a suitable partial differential equation in spatial dimension 1, containing a weight depending on  $\alpha$ .

The limiting cases  $\alpha = 0$ ,  $\alpha = 1$  are also considered.

- In [3] we look at the case where nonlinear convection is present in the equation, more specifically at the case

$$\frac{\partial u}{\partial t} - \operatorname{div}(\nabla u^m) = -\frac{\partial u^m}{\partial x_N}, \quad \text{in } \mathbf{R}^N \times (0, +\infty),$$

with  $m > 1$ ,  $N \geq 2$ . The 1-dimensional case was known. We prove for solutions with integrable initial data the sharp decay rate corresponding to the negative power  $-(N+1)/[(N-1)(m-1)+2m]$ , which is faster than the case without convection. The difficulty here is the anisotropy in the differential equation, which we exploit resorting to a kind of weak entropy inequality.

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## M-22. Integro-differential models & Materials with memory: viscoelasticity and magneto-viscoelasticity

S. Carillo

The name *materials with memory* is introduced to identify 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. In this framework, the Volterra viscoelasticity equation reads

$$\mathbf{u}_{tt} - \mathbb{G}(0)\Delta\mathbf{u} + \int_0^t \dot{\mathbb{G}}(t-\tau)\Delta\mathbf{u}(\tau)d\tau = \mathbf{f} \quad (1)$$

where  $\mathbf{u}$  denotes the displacement and  $\mathbb{G}$  the relaxation modulus which plays the role of the memory kernel. The history of the material as well as an external force, if present, are included in the term  $\mathbf{f}$ . The *classical* assumptions on relaxation modulus in (1) prescribe

$$\mathbb{G} \in L^1(\mathbb{R}^+) \quad , \quad \dot{\mathbb{G}} \in L^1(\mathbb{R}^+, Lin(Sym)) \quad (2)$$

so that

$$\mathbb{G}(t) = \mathbb{G}_0 + \int_0^t \dot{\mathbb{G}}(s) ds \quad , \quad \mathbb{G}(\infty) = \lim_{t \rightarrow \infty} \mathbb{G}(t) \quad , \quad (3)$$

where  $\mathbb{G}(\infty) \in Lin(Sym)$  is termed *equilibrium elastic modulus*. Furthermore, the relaxation modulus  $\mathbb{G}$  enjoys the *fading memory property*, that is,  $\forall \varepsilon > 0$  it exists  $\tilde{a} = \tilde{a}(\varepsilon, \mathbb{E}^t) \in \mathbb{R}^+$  such that

$$\forall a > \tilde{a}, \quad \left| \int_0^\infty \dot{\mathbb{G}}(s+a)\mathbb{E}^t(s) ds \right| < \varepsilon. \quad (4)$$

The physical meaning of the fading memory property is that, at the present time, the effect of the very far away in time deformations is negligible.

The research project is concerned about generalisations of the *classical* model to describe the behaviour of new materials; thus, the classical regularity assumptions (5) on the kernel  $\mathbb{G}$  are relaxed. Specifically, (5) is replaced by the weaker

$$\mathbb{G} \in L^1(\mathbb{R}^+) \quad , \quad (5)$$

which allows to consider  $\mathbb{G}$  unbounded at  $t = 0$ . The existence and, possibly, uniqueness of the admitted solutions to initial boundary value problems is studied. The materials with memory considered are isothermal viscoelastic bodies as well as rigid heat conductors with memory. Subsequently, the effects of linear viscoelasticity are coupled with magnetic ones. This allows to model new materials such as, for instance, magneto-sensitive polymeric composites whose viscoelastic behaviour is singular. In particular, the results obtained during the time period 2015-17 can be listed as follows:

- Non-classical memory kernels in linear viscoelasticity are studied in [1] where the model of viscoelastic body is described aiming to extend their validity to a wider class of materials. In particular, *aging* effects which change the mechanical response of viscoelastic materials with time.
- The case of singular kernel problem is studied in [1] where different materials with memory are considered. Rigid heat conduction with memory as well as isothermal viscoelasticity problems are analysed in the case of a singular kernel integro-differential model equations; that is when, respectively, the heat flux relaxation function, and the relaxation modulus, are unbounded at  $t = 0$ . Similarities and discrepancies between the two cases are discussed.
- In [3] an existence result is obtained in the case of a three-dimensional viscoelastic body characterised by an relaxation modulus unbounded at  $t = 0$ . This result generalises a previous one in collaboration with V. Valente, G. Vergara Caffarelli.
- Magneto-viscoelasticity problems are considered in [4] where the existence existence of solutions admitted by a one-dimensional is proved. The generalised case of the coupling between magnetic effects and singular viscoelasticity is studied.
- In [5] regular kernel as well as singular kernel viscoelasticity materials subject to the effect of magnetisation are discussed.
- Currently, a further generalisation is under investigation and the one-dimensional results obtained are in [6]. In this case a bounded, continuous relaxation function which admits a discontinuous derivative is studied.

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## M-23. Effects of spatial heterogeneities on mass transport

*E.N.M. Cirillo, D. Andreucci*

In the framework of the Statistical Mechanics and Stochastic Particle System research line, a great effort has been made in the recent years towards the understanding of particle flows in presence of obstacles.

Barriers can either speed up or slow down the dynamics: obstacles can induce a sub-linear behavior with respect to time of the mean square distance traveled by Brownian particles. This *anomalous diffusion* is observed in cells and explained as due to macromolecules playing the role of obstacles for smaller molecules. On the other hand, it has been proven that the presence of an obstacle can accelerate the dynamics in granular system where the out-coming flow, reduced by the clogging at the exit, can be improved by placing an obstacle above it. A similar phenomenon is observed in pedestrian flows in case of fast egress. These phenomena are a sort of inverse *Braess' paradox*: adding a road link to a road network can cause cars to take longer to cross the network, adding barriers results in a decrease of the time that particles need to cross a region of the space.

We have attacked these phenomena in a very basic scenario: the effect of the barriers on the typical time, the *residence time*, that a particle needs to cross a 2D strip is evaluated for different simple dynamics such as the *simple symmetric random walk*, the *simple exclusion model* and the *linear Boltzmann dynamics*.

The residence time issue has been posed in [4] for a particle flow undergoing a random walk with exclusion in an horizontal strip. 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 using Monte Carlo simulations and analytic tools. It has been shown that, in some regimes, the residence time is not monotonic with respect to the size of the obstacle. This complex behavior has been related to the way in which particles are distributed along the strip at stationarity, namely, to the occupation number profile, which, in turn, strongly depends on the way in which particles interact due to the presence of the exclusion rule.

In [2] we considered the same geometry for the linear Boltzmann dynamics: a particle moves along a line with constant velocity for an exponential random time, then it changes the direction of its motion simulating the hit with a circular scatterer. Even in this independent particle model surprising behaviors are found: the residence time is non-monotonic with respect to the side lengths of the obstacle and its position. In some cases, the residence time 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 with respect to the empty strip case. This complex behavior is not intuitive at all. Similar behaviors are found for particles performing independent

random walks on a 2D strip: if the linear Boltzmann dynamics is observed on a larger space scale, its behavior is similar to the one of a two dimensional random walk.

These phenomena are due to 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.

A 1D random walk model mimicking the 2D geometry has also been studied: behaviors similar to those observed in 2D are found via exact and Monte Carlo computations. The role of the obstacle is played by *defect* sites. Not monotonic behaviors of the residence time as a function of the position of the defect and the probability of a right jump for a particle at the defect are found (Figure 1).

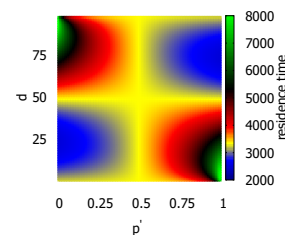


Figure 1: Residence time as a function of the position of the defect site  $d$  and the right jump probability  $p'$ .

Other problems connected to this research line have been attacked in 1D and 2D: we have studied the possibility of inducing not Fickian currents in 1D systems [3] adding a single defect to a conducting lane and we have derived, starting from a microscopic lattice model, in the hydrodynamic limit both the Fick and the Fokker-Planck diffusion equations by introducing site or edge heterogeneities [1].

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## M-24. Controllability of evolutive equations

*P. Loreti*

In the period 2015-2107 we addressed the following main topics concerns controllability:

- Discrete and continuous models for hyper-redundant architecture.

Hyper-redundant architecture was intensively studied back to the late 60's. The interest of researchers in devices with redundant controls is motivated by their ability to avoid obstacles and to perform new forms of robot locomotion and grasping. A research on control dynamics of bio-inspired systems modeling animal arms as a sequence of interacting links, with approaches from a discrete to a continuous setting is under going. These works go in the directions to combine number theory and discrete mathematics to model an arbitrary precision in a robot. Then a continuous model may be obtained. Expansions in non-integer bases and Fibonacci numbers may be used.

With respect to this topic, see paper [1].

- Expansions in non-integer bases.

Some questions above are particular cases of a subject of theoretic interest in expansions in non-integer bases. In [2] Cantor's ternary function is generalized to arbitrary base-change functions in non-integer bases. Also it have been studied topological and combinatorial properties of the set of univoque bases and their corresponding sequences.

- The Fourier method in control problems

Fourier method is used for the study of different evolutionary systems. A general Fourier type approach was developed for control systems that are of common use such as plates, beams, membranes, strings, and systems of them. The method apply to many different boundary conditions for which the associated eigenfunctions have suitable explicit forms for the application of Fourier series. For the investigation of higher dimensional problems finer properties of some special functions as the distribution of zeros of Bessel's functions, had to be established. Controllability and observability by the Fourier method are based on a generalization of Parseval's formula of the trigonometrical system to more general families of exponentials. Ingham's theorem extended the analysis to sets of real numbers satisfying a uniform gap condition. This leads to obtain observability inequalities and controllability results for a class of partial differential equations and for coupled systems. The interaction is studied by an asymptotic spectral analysis, and an estimate of the asymptotic gap. Applications are also investigated

With respect to this topic, see paper [3].

- Viscoelastic materials and related problems.

The memory leads to study controllability of partial differential equations with integro-differential terms, and their coupling. The method to answer to controllability questions makes use of tools from harmonic analysis. It gives precise estimations of the controllability time.

Control and inverse problems for isotropic and anisotropic materials lead to study integro-differential equations. The viscoelastic material is also described by the kernel function. Also Carleman estimates for the integro-differential operator are obtained in [5], the result is based on Carleman estimates for the parabolic equation, and the integral kernel has a behaviour like a weakly singular one.

See [4], [5], [6].

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## M-25. Bäcklund transformations & nonlinear operator equations on Banach spaces: structural properties and applications

*M. Lo Schiavo, S. Carillo*

Bäcklund transformations represent a very powerful tool to investigate nonlinear evolution equations which admit so called *soliton solutions*. The long lasting research project, is concerned about various applications of Bäcklund transformations. The main research lines are the following ones: - Establish links among nonlinear evolution equations via Bäcklund transformations.

- Deduce algebraic properties they enjoy.
- Extend the results to corresponding hierarchies.
- Construct admitted solutions.
- Generalize the study from real to operator valued unknowns.

By Bäcklund transformation is meant a relation, generally nonlinear, which connects solutions of two different nonlinear evolution equations. Specifically, given the two nonlinear evolution equations  $u_t = K(u)$  and  $v_t = G(v)$ , they are linked via the Bäcklund transformation  $B(u, v) = 0$ , when, given any solution  $u(x, t)$  of the first equation, it turns out to be connected to a solution, say  $v(x, t)$ , of the second one. That is, if  $B(u, v)|_{t=0} = 0$  it follows that  $B(u, v) = 0, \forall t$ . The importance of Bäcklund transformations is twofold since they, on one side, allow to construct solutions of nonlinear evolution equations from solutions of other ones via the established connections. On the other side, also many algebraic properties are preserved under Bäcklund transformations. When various nonlinear evolution equations are all connected via Bäcklund transformations, the net of links can be summarized in a *Bäcklund chart*.

When a nonlinear evolution equation is proved to admit a hereditary recursion operator, then, all the nonlinear evolution equations connected to it via Bäcklund transformations can be proved to enjoy the same remarkable property. Indeed, the recursion operators allows to construct the corresponding hierarchies. Then, the links are extended to the whole hierarchies. The results obtained during the time period 2015-17 can be listed as follows:

- Construction of a wide operator Bäcklund chart which involves 3rd order nonlinear evolution equations as well as the corresponding hierarchies [1].
- The operator Bäcklund chart is further extended in [2] where new operator equations are obtained together with the admitted recursion operators and, hence, the corresponding hierarchies.
- In [3] analogies and discrepancies between the cases of real valued unknowns, on one side, and operator unknowns, on the other, is exploited. In addition, the Bäcklund chart connecting nonlinear evolution

equations in with real valued unknowns, previously obtained, is further extended.

- In [4] the recursion operators admitted by different operator Burgers equations, in which the unknown is an operator acting on a Banach space are investigated. The mirror non-Abelian Burgers equation  $r_t = r_{xx} + 2r_x r$  is considered. The structural properties of the admitted recursion operator are studied.
- Bäcklund transformations are applied to construct solutions admitted by physically interesting problems in [5,6], where, respectively, the Ermakov-Pinney and Emden-Fowler equations, and the Gross-Pitaevskii equation are investigated.
- Currently, explicit solutions admitted by modified Korteweg de Vries (mKdV) matrix equations are under investigation by S. Carillo, M. Lo Schiavo, C. Schiebold. Previous results are applied in the particular case when the operator is finite dimensional and, hence, can be represented by a matrix. An example of an obtained result is in Fig. 1.

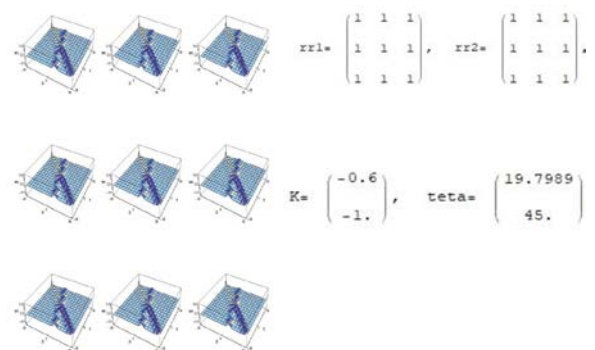


Figure 1: Solution of a 3x3 matrix mKdV equation.

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## M-26. Brain Imaging by MEG/EEG data

*F. Pitolli, B. Vantaggi*

Neuroimaging aims at reconstructing the neuronal activity generated in the working brain using, for instance, Electroencephalography (EEG) and Magnetoencephalography (MEG). These non-invasive techniques 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. Thus, by using MEG/EEG it is possible to study non-invasively the brain at work and to diagnose possible pathologies such as, e.g., epilepsy.

From the mathematical point of view, to reconstruct the brain activity map from MEG and EEG data we need to solve a highly ill-posed and ill-conditioned inverse problem that requires cutting edge mathematical inversion methods.

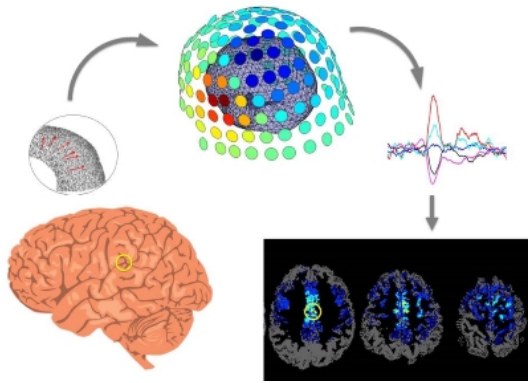


Figure 1: Reconstruction of the brain activity map by MEG signals.

We implemented an efficient algorithm, the Iterative Alternating Scheme (IAS) [1-3], that is able to reconstruct accurately the electric activity map in the brain by MEG/EEG signals.

### The IAS Algorithm

1. Initialize  $\theta = \theta^0$ , and set  $k = 0$
2. Update  $Q$  with fixed  $\theta = \theta^k$ :

$$Q^{k+1} = \operatorname{argmin} \left\{ \frac{1}{2} \|b - MQ\|_{\Sigma}^2 + \frac{1}{2} \|Q\|_{D_{\theta^k}}^2 \right\}$$

where  $C_{\theta} = \operatorname{diag}(\theta_1 C_1, \dots, \theta_n C_n)$ ,  $D_{\theta}^T D_{\theta} = C_{\theta}$

3. Update  $\theta$  with fixed  $Q = Q^{k+1}$ :

$$\theta_j^{k+1} = \theta_j^* \left( \frac{\eta_j}{2} + \sqrt{\frac{\eta_j^2}{4} + \frac{\|\bar{q}_j^{k+1}\|_{C_j}^2}{2\theta_j^*}} \right), \eta_j = \beta_j - 5/2$$

4. If a convergence criterion is met, stop, else increase  $k$  by one and continue from Step 2

The algorithm learns from the data the main features of the neural sources responsible for the measured magnetic field and is particularly suitable for the characterization of the activity of deep brain sources and, thus, useful both in clinical diagnosis and in neuroscience study targeted at subcortical brain areas [4].

A slimmer inversion method useful in real-time applications can be found in [5].

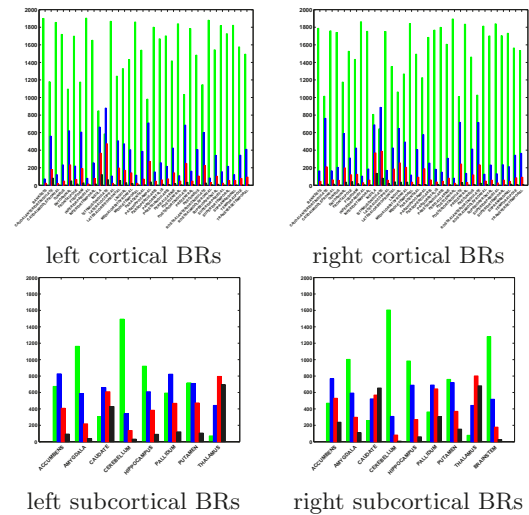


Figure 2: Bayes factor analysis of the reconstructed brain activity by the IAS algorithm: The prevalence of green and blue bars (Bayes factor above 10 and in the interval  $[3, 10]$ , respectively) indicates that the activity has been detected in the correct brain region (BRs).

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## M-27. Integro-differential equations: well-posedness and controllability

*D. Sforza, P. Loreti*

The main studies performed in the period 2015-2017 in the area of integro-differential equations can be summarized as follows.

- In [1] we deal with a coupled system obtained by combining a wave equation with viscoelastic damping and a Petrovsky type equation. Under suitable assumptions involving the parameters of the memory kernel, which is of exponential type, partial observability inequalities for the first and the second components are obtained. The results are proved by using non-harmonic analysis techniques.
- In [2] we show a reachability result for the solution of a multidimensional coupled Petrovsky and wave system when a non local term, expressed as a convolution integral, is active. Motivations to the study are in linear acoustic theory in three dimensions. To achieve that, we prove observability estimates by means of Ingham type inequalities applied to the Fourier series expansion of the solution.
- The paper [3] is devoted to prove a "hidden regularity" result for a model of integro-differential equations in which the integral term is of convolution type with a nonnegative kernel satisfying suitable assumptions that yield a nonincreasing energy of the weak solution to the problem. In fact, the result concerns the definition of the trace of a weak solution of an integro-partial differential equation and is a generalization of well-known results about wave equations without memory.
- The Hilbert Uniqueness Method introduced by J.-L. Lions in 1988 has great interest among scientists in the control theory, because it is a basic tool to get controllability results for evolutive systems. In [4] our aim is to outline the Hilbert Uniqueness Method for first order coupled systems in the presence of memory terms in general Hilbert spaces. At the end of the paper we give some applications of our general results.
- On the basis of the Carleman estimate for the parabolic equation, in [5] we prove a Carleman estimate for the integro-differential operator  $\partial_t - \Delta + \int_0^t K(x, t, r)\Delta dr$  where the integral kernel has a behaviour like a weakly singular one. In the proof we consider the integral term as a perturbation. The crucial point is a special choice of the time factor of the weight function.
- In [6] we consider an anisotropic hyperbolic equation with memory term, which is a simplified model

equation for viscoelasticity. The main result is a both-sided Lipschitz stability estimate for an inverse source problem of determining a spatial varying factor of the force term. The proof is based on a Carleman estimate and due to the anisotropy, the existing transformation technique does not work and we introduce a new transformation of the solution in order to treat the integral terms.

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## M-28. Perturbative methods and concentration phenomena in nonlinear problems

*A. Pistoia*

This line of research aims at investigating concentration phenomena for a large class of elliptic nonlinear partial differential equations (PDEs for short) of interest in physical and geometrical applications. There is a definite interest in concentrated quantities, useful to model for instance the wave-function of a particle in the semi-classical limit or a turbulent fluid in presence of vortices. Perturbative parameters are completely natural in this context and simply correspond to particular physical regimes. To support concentration phenomena, the involved PDEs present intrinsic invariances which are possibly responsible for a lack of compactness, making their analysis very subtle. A crucial role in the analysis is played by the classification of entire solutions in the whole space, an investigation of their symmetry properties and their degeneracy. The study of entire solutions to semilinear elliptic PDEs is an area of investigation with long tradition. The research aims to shed new light on frontier topics concerning such critical nonlinear PDEs, by exploiting a powerful constructive approach of perturbative type, whose flexibility led in recent years some major breakthrough advancement, like the construction of counter-examples in large dimension to the De Giorgi's conjecture and to the Schoen's conjecture on compact non-locally conformally Riemannian manifolds. In particular, the research have been focusing on selected problems in the following fields:

(i) Liouville type problems.

In 1853 Liouville introduced the following equation  $\Delta u + e^u = 0$  in  $D$ , where  $D$  is a regular 2-dimensional domain (possibly the whole plane). This problem has been a great source of inspiration for important ideas in different branches of mathematics. It is also mentioned in the formulation of the nineteenth Hilbert problem We study a class of two-dimensional elliptic PDEs involving exponential nonlinearities, in the scalar case as well as in the case of systems. We are concerned with existence and uniqueness issues in some special regimes, with special attention to the classical Liouville equation. (see e.g. [1], [2])

(ii) Conformal geometric problems.

Given  $(M, g)$  a smooth, compact Riemannian manifold of dimension  $N \geq 3$ , the prescribed scalar curvature problems consists in finding a metric conformal to  $g$  whose scalar curvature is a given function. In particular, the Yamabe problem consists in finding metrics of constant scalar curvature in the conformal class of  $g$ . These problems turn out to be equivalent to finding a positive solution to a PDE with critical growth on the manifold. We study the

existence, stability and compactness of solutions to a class of Yamabe type problems on manifolds with or without boundary (see e.g. [3], [4]).

(iii) Competitive systems.

Another example where geometric structures appear are systems of elliptic equations for competing species. Several physical phenomena can be described by a certain number of densities (of mass, population, probability, . . . ) distributed in a domain and subject to laws of diffusion, reaction, and competitive interaction. Whenever the competitive interaction is the prevailing phenomenon, the several densities cannot coexist and tend to segregate, hence determining a partition of the domain. We focus on the existence and the analysis of qualitative properties of solutions to systems of semilinear elliptic equations with strong competitive interactions (see e.g. [5], [6])

The research group include leading worldwide experts in nonlinear partial differential equations as well as junior researchers and students.

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## M-29. Spectral and geometric analysis on Riemannian manifolds

A. Savo

Spectral Geometry investigates relationships between geometric structures of Riemannian manifolds and spectra of various elliptic operators. Our research in the period 2015-17 focused on the following topics:

- Overdetermined problems for the heat equation
- Eigenvalue estimates for the weighted Laplacian and the biharmonic Steklov problem

In Riemannian geometry, an overdetermined problem gives rise to the following question: is it possible to identify the geometry of a domain  $\Omega$  in a Riemannian manifold assuming the existence of a solution  $u$  of a certain PDE such that both  $u$  and its normal derivative are constant on the boundary of  $\Omega$ ? Perhaps the most famous example of overdetermined problem is the so-called *Serrin problem* :

$$\begin{aligned} \Delta v &= 1 & \text{on } \Omega, \\ v &= 0, \quad \frac{\partial v}{\partial \nu} = c & \text{on } \partial\Omega. \end{aligned} \quad (1)$$

J. Serrin celebrated rigidity result, which dates back to 1971, states that the only compact Euclidean domains supporting a solution to (1) are Euclidean balls. One could ask if a similar rigidity theorem holds in more general Riemannian manifolds. Well, the answer is negative: already in a manifold as basic as the standard sphere  $\mathbf{S}^n$  there are *exotic* domains (that is, domains not isometric to geodesic balls) which support solutions to the overdetermined problem (1): examples are given by domains bounded by isoparametric hypersurfaces, a class of hypersurfaces whose study goes back to Cartan. The question is then the following : does the class of isoparametric domains exhaust all possible solutions to (1)? The answer is again negative as shown in a recent work by Fall, Minlend and Weth, where even more exotic examples are constructed. Thus, at the moment, a classification seems out of reach even in "simple spaces" as round spheres.

In our work, we considered a related problem as follows. Let  $u(t, x)$  be the solution of the heat equation on a Riemannian domain  $\Omega$ , with unit initial conditions ( $u(0, x) = 1$  for all  $x \in \Omega$ ) and Dirichlet boundary conditions ( $u(t, y) = 0$  for all  $t > 0$  and  $y \in \partial\Omega$ ). Then it is well-known that the solution exists and is unique. We say that  $\Omega$  has the *constant flow property* if the normal derivative of the solution is constant on the boundary at any fixed time. This request is met by highly symmetric domains, but not only: in the sphere, it is also met by domains with isoparametric boundary, which do not always have homogenous boundaries. Moreover, it is easy to show that any domain with the constant flow property automatically supports a solution to (1); in fact, the

constant flow property is stronger than the property in (1), and then there is hope for a classification. This is what we do in our papers [3] and [4]. In our paper [3] we show, in particular, that a spherical domain with connected boundary has the constant flow property if and only if its boundary is in fact isoparametric, thus giving a classification result. In our recent paper [4] we refined and extended the above results to show that, more generally, a domain in an analytic Riemannian manifold has the constant flow property if and only if it is an *isoparametric tube*, in the sense that it is a smooth tube around a smooth, closed, minimal submanifold  $N$  with the property that every equidistant to  $P$  has constant mean curvature.

In conclusion, we obtained a classification of analytic manifolds with the constant flow property, and this result gives a new analytic characterization of the isoparametric property.

A central problem in Spectral Geometry is to estimate eigenvalues of elliptic operators acting on manifolds in terms of geometry. In [1] we study the Laplacian acting on a compact manifold endowed with a smooth density  $f dv_g$ , where  $dv_g$  is the Riemannian measure and  $f$  is a positive function. The resulting operator is called in the literature Bakry-Émery or also Witten Laplacian. We prove upper bounds for the  $k$ -th eigenvalue which are consistent with the right power of  $k$  in Weyl's formula, and depend on integral norms of the density  $f$ , instead of pointwise norm as in previous works.

In [2] we studied the biharmonic Steklov eigenvalue problem on a compact manifold with boundary, first introduced in classical works by Kuttler and Sigillito. We give a sharp lower bound of the first eigenvalue which improves known estimates; in particular, we obtain a sharp lower bound for the isoperimetric ratio of positive subharmonic functions.

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# Research Activities: Physics

# Physics - Introduction

SBAI research in Physical Sciences concerns a number of different areas, with a common focus on issues exhibiting significant potential applications. On each topic, however, application-oriented activities are supported and complemented by theoretical, computational and experimental basic research. This two-faceted approach emerges clearly from the following brief one-page reports outlining the activities carried on in the years 2015-2017. These summaries show that individual research topics are clustered around a few transversal themes, with significant links and intersections with each other. Furthermore, most activities are performed within the frames of large national and international collaborations, as well as taking advantage from the large net of research institutions based in or around Rome. The resulting panorama is that of a timely research well integrated in the international panorama, exploiting a unique set of expertise, and profiting from its integration in an Engineering school.

This rich network of activities makes any classification and grouping of research themes rather arbitrary and, in any case, partial and incomplete. Following a traditional scheme, we find investigations on electromagnetism, classical and quantum optics, acoustics, condensed matter, plasma physics, nuclear physics, spectrometry. But such a sorting would in most case hide SBAI research goals and SBAI uniqueness within Sapienza. Indeed, the focus of our physics research is better evidenced by considering the areas of application. These include development and characterization of innovative materials (such as nano-structures or meta-materials), applications of non-linear optics and plasmonics, a wide spectrum of bio-medical applications (including bio-sensing, adrotherapy, ultrasound diagnostics), advanced acceleration techniques, energy applications, archaeometry, radiation protection. Worth noticing, most of the above areas leverage on the development of non-destructive diagnostics, based on acoustic, thermal, optical, X-ray, nuclear detectors. Innovative computational activities are also performed, especially in the areas of plasma physics, nanomaterials and adrotherapy.

A significant fraction of SBAI experimental research in Physics is conducted in the Department Laboratories. These laboratories (with the instrumentation described in Sec. x) are also available to the Sapienza community, and more generally, to interested outside researchers. For investigations requiring larger facilities SBAI groups utilize, in the frame of appropriate collaborations, national and international facilities, such as those at INFN, CNR, CINECA, CERN, GSI, and in the LaserLab consortium.

# Physics - List of research activities

- P-1. High brightness beams for novel particle accelerators
- P-2. Beam dynamics and instabilities in future accelerators
- P-3. Longitudinal and transverse wakefields simulations and studies in dielectric-coated circular waveguides
- P-4. Online monitoring of carbon ions particle therapy treatments
- P-5. FragmentatiOn Of Target (FOOT) studies
- P-6. Fast dose recalculation on GPU for particle therapy applications
- P-7. MONDO (MOnitor for Neutron Dose in hadrOntherapy)
- P-8. New Organic Scintillators
- P-9. Biomedical ultrasonics
- P-10. Elastic guided waves
- P-11. Laser-driven inertial confinement fusion and high energy density plasma physics
- P-12. Kinetic and hybrid simulations of plasma-based accelerators and plasma lenses
- P-13. Laser-Accelerated Proton Beams as Diagnostics for Cultural Heritage
- P-14. Laser physics for particle accelerators and radiation sources
- P-15. Electron Microscopies and Nanoscopies (EMINA)
- P-16. Density Functional Theory and beyond: surface, bulk and optical properties of materials and nano-structures
- P-17. Plasmonics and photonics : linear and nonlinear optical properties of metamaterials and metasurfaces
- P-18. Characterisation of nanostructures by second harmonic generation
- P-19. Multipolar nano antennas for tailored infrared thermal emission and nanoscale radiative heat transfer
- P-20. Infrared radiation manipulation in polar metamaterials
- P-21. Nondestructive testing by photoacoustic and photothermal techniques
- P-22. Molecular photonics: from linear and nonlinear optics in organic materials to biophotonics and liquid biopsy
- P-23. Cognitive- and bio-photonics
- P-24. Non-destructive analyses and archaeometry
- P-25. Radiation protection

## P-1. High brightness beams for novel particle accelerators

*A. Mostacci, L. Ficcadenti, M. Migliorati, M. Petrarca, L. Palumbo*

Particle accelerators are widely used tools for industry, medicine and science. Today there are some 30,000 particle accelerators worldwide, all relying on long-proven and highly developed methods for particle acceleration. The possible energy of particles is often limited by practical boundaries on size and cost, for example, the available space in hospitals, the available university funding for accelerator-based light sources or the cost society as a whole can afford for science projects at the energy frontier. Novel acceleration methods with plasma-based structures have demonstrated acceleration of charged particles in a length reduced by a factor 100-1000. The electron pulses from plasma accelerators are short (few femto-seconds) and open a ground-breaking route into novel applications for ultra-fast science. Similar high-brightness electron beams are nowadays used for many applications such as, for instance, the generation of THz and free-electron laser (FEL) radiation, inverse Compton scattering and transmission electron microscopy.

This research is conducted at the SPARC.LAB facility at INFN Frascati National Laboratory (INF-LNF) hosting a high brightness photo-injector used to drive Free Electron Laser experiments and explore advanced beam manipulation techniques. The R&D aims to the generation and optimisation of sub-picosecond, high brightness electron bunch trains via RF compression at few MeVs energy. Such bunch trains can be used to drive tunable and narrow band THz sources, FELs and plasma wake field accelerators for few femto-seconds beams.



Figure 1: SPARC.LAB high brightness linear accelerator.

Even though the principle of plasma-based acceleration has been proven by several groups, the so accelerated beams still suffer from large angular divergence, large energy spread, poor reproducibility, which prevent their use as an alternative to conventional RF accelerators which typically provide stable and high quality electron beams. Our approach towards plasma-accelerated high-brightness electron beams relies on the use of the

plasma only as the active media, injecting electrons into a pre-formed plasma channel. A first scheme consists in injecting a witness electron bunch in a plasma where the plasma wave is excited by a high-power laser pulse. A second scheme relies on the induction of coherent plasma oscillations with multiple electron bunches. In parallel to the demonstration of compact, reliable, plasma wake field acceleration, one has also to foresee new focusing devices with tiny sizes. So far, permanent-magnet quadrupoles represent the state of the art providing focusing gradients of the order of 600 T/m. Nevertheless, their focusing is nonsymmetric and the gradient fixed thus nontrivial movable systems (consisting of at least three lenses) must be implemented to produce round beams with (slightly) adjustable focal length.

An active-plasma lens is a few cm long capillary filled by  $H_2$  gas able to symmetrical focus the beam while preserving the beam emittance. Increasing the discharge current flowing through the capillary and with a proper bunch shaping, the detrimental effects induced on the beam dynamics are minimized. Once tuned, the system (see Fig. 2) allowed us to reach a strong focusing that resulted in a beam waist of  $17 \mu\text{m}$  and minimal increase of the horizontal beam emittance, although the growth is more pronounced on the vertical plane. It is worth pointing out that the preservation of the beam emittance is a key requirement for high-brightness beams and our results represent thus a fundamental step toward the development of next-generation focusing optics and demonstrate their effective usability in view of new compact accelerators where both focusing and acceleration can rely on properly excited plasmas.

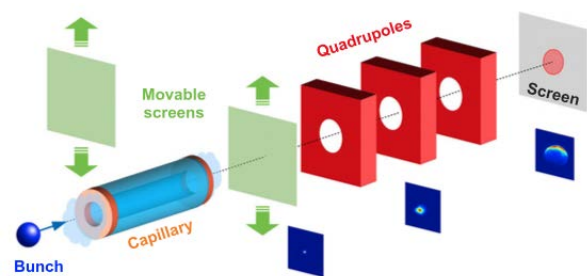


Figure 2: Focusing of High-Brightness Electron Beams with Active-Plasma Lenses: experimental layout [1].

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## P-2. Beam dynamics and instabilities in future accelerators

*M. Migliorati, A. Mostacci, L. Palumbo*

The European Organization for the Nuclear Research (CERN), is one of the world's largest centres for scientific research. The main accelerator of the CERN's laboratory is the Large Hadron Collider (LHC). It first started up on 10 September 2008, and remains the latest addition to CERN's accelerator complex. The LHC consists of a 27-kilometre ring of superconducting magnets with a number of accelerating structures to boost the energy of the particles along the way.

On 4 July 2012, the ATLAS and CMS experiments at LHC announced they had each observed a new particle in the mass region around 126 GeV. This particle is consistent with the Higgs boson predicted by the Standard Model. Thanks to this discovery, on 8 October 2013 the Nobel prize in physics was awarded jointly to François Englert and Peter Higgs.

LHC, which is unlike any other particle accelerator, is now just at the start of a new programme which is expected to run for another 20 years in the framework of the High-Luminosity Large Hadron Collider (HL-LHC) project, which aims to improve the performance of the LHC in order to increase luminosity by a factor of 10 beyond the LHC's design value.

The LHC upgrade programme is currently well defined for the next two decades. However physicists and engineers look even further ahead, and CERN is starting an exploratory study for a future long-term project centred on a new generation of circular colliders with a circumference of about 100 kilometres. This new collaboration study is called Future Circular Collider (FCC) study, and it comprises a hadron collider in the same tunnel of LHC, capable of reaching an energy of 27 TeV based on 16 tesla superconducting magnets, a more large hadron collider of about 100 km with unprecedented energies in the region of 100 TeV (FCC-hh), and a high-luminosity  $e^+e^-$  collider (FCC-ee) in the same 100 km tunnel.

In Fig. 1 a schematic map shows where the Future Circular Collider tunnel is proposed to be located with respect to the existent LHC tunnel.

These new accelerators (HL-LHC, FCC) require beams of high intensity which, interacting electromagnetically with the vacuum chamber and all the machine devices, generate strong electromagnetic fields, known as wakefields, that act back on the beam and can lead to instabilities with subsequent beam losses. 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.

Our group has a long tradition in the field of beam dynamics, wakefields, instabilities and collective effects, and it has developed tools for analytical and numerical

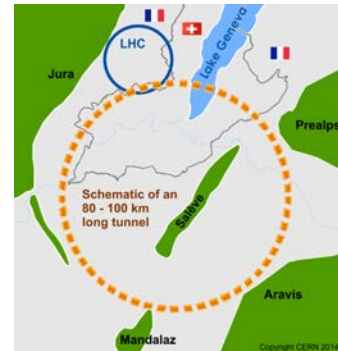


Figure 1: A schematic map showing the FCC and LHC tunnels in the Geneva area.

studies of longitudinal and transverse instabilities in particle accelerators [1]. In the years 2015-17 the group has been responsible of the work on collective effects in FCC-ee and is participating to the writing of the Conceptual Design Report. Moreover, different collaborations with CERN are related to the study of collective effects for the upgrade program of LHC and its injectors chain.

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, during this design study phase, 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. This machine represents a great challenge with unprecedented requests in terms of beam intensities, and this important work on collective effects is still in progress. Finally, for the upgrade project of LHC, we have been involved, in particular, on wakefields and instabilities for the CERN PS [2], one of the LHC injectors which is responsible of the longitudinal characteristics of the LHC beams in the HL-LHC project. A model taking into account the wakefields generated by several sources in the machine has been developed and many direct beam measurements on the PS have been performed to validate the model, which represents now a reliable tool for the study of the collective effects for this machine. The same approach is being applied to other injectors and to HL-LHC.

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### P-3. Longitudinal and transverse wakefields simulations and studies in dielectric-coated circular waveguides

*L. Ficcadenti, G. Castorina, D. Francescone, M. Marongiu, M. Migliorati, A. Mostacci, A. Biagioni, L. Palumbo*

In recent years, there has been a growing interest and rapid experimental progress on the use of e.m. fields produced by electron beams passing through dielectric-lined structures and on the effects they might have on the drive and witness bunches. Short ultra-relativistic electron bunches can excite very intense wakefields, which provide an efficient acceleration through the dielectric wakefield accelerators (DWA) scheme [1] with higher gradient than that in the conventional RF LINAC. These beams can also generate high power narrow band THz coherent Cherenkov radiation. These high gradient fields may create strong instabilities on the beam itself causing issues in plasma acceleration experiments (PWFA), plasma lensing experiments and in recent beam diagnostic applications. We have studied the wakefields generated by electron beams at different lengths and charges passing on-axis and off-axis in dielectric-coated circular waveguides. The beam driven dielectric wakefield accelerators (DWFA) make use of the electromagnetic Cherenkov radiation (wakefield) [2] from the electron bunches that pass through the dielectric-lined waveguides (DLW). Particle In Cell (PIC) simulations can be

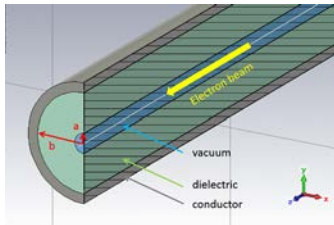


Figure 1: DLW geometry

performed with CST Microwave Studio package. An example of study is represented in Fig. 1. The outer radius is  $b = 2.5$  mm, the circular waveguide is filled, from the radius  $a = 0.5$  mm to the outer radius, with a perfect dielectric material of dielectric constant  $\epsilon_r = 4.82$ , the external conductor is loss free. The length of the structure is about 100 mm. We considered gaussian electron beams of different lengths and different charges, we explored longitudinal dimensions that goes from  $\sigma_z = 1$  mm to  $\sigma_z = 0.1$  mm and charges from 50 pC to 200 pC. The electron beam energy is  $E = 126$  MeV, the transverse dimension of the beam is that of the metal cathode which must be defined in the PIC simulations. We have chosen a beam transverse dimension of  $\sigma_t = 0.15$  mm. Fig 2 shows the absolute value of the electric field inside the dielectric guide when the electron beam has almost reached the exit of the structure, after  $t = 0.29$  ns from the cathode emission (left part). Fig. 3 shows the lon-

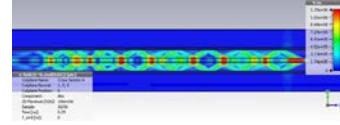


Figure 2:  $|E|$  behind the electron beam, inside the DLW, at time 0.29 ns, when the beam is at  $z = 80$  mm.

gitudinal electric field ( $E_z$ ) on the axis behind the electron beam for different values of the total charge (50 pC, 100 pC and 200 pC), keeping the longitudinal dimension of the beam fixed at  $\sigma_z = 1$  mm. Fig. 4 shows the

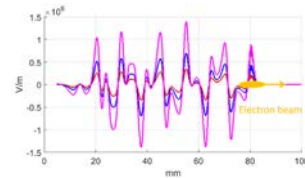


Figure 3:  $E_z$  behind the electron beam, after  $t = 0.29$  ns from the cathode emission, for different beam total charges: 50 pC (red); 100 pC (blue); 200 pC (magenta).

longitudinal electric field ( $E_z$ ) for 50 pC charged beam for different longitudinal dimensions  $\sigma_z$  (1 mm, 0.5 mm, 0.3 mm and 0.1 mm). The effects of the beam shortening are substantially two: the field amplitude is inversely proportional respect the beam length [1] and the field on axis tends to concentrate at a distance determined by the thickness of the dielectric ( $b - a$ ). For shorter electron beams the longitudinal electric field assume a spike shape, presenting zones with a high accelerating gradient. For these structures, using 0.1 mm long beams, electric fields of the order of some MV/m are reached.

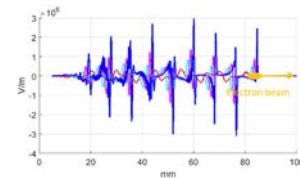


Figure 4:  $E_z$  behind the electron beam, at  $t = 0.29$  ns, for different  $\sigma_z$ : 1 mm (red) line; 0.5 mm (cyan); 0.3 mm (magenta) and 0.1 mm (blue).

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## P-4. Online monitoring of carbon ions particle therapy treatments

*A. Sarti, M. De Simoni, M. Fischetti, M. Magi, M. Marafini, R. Mirabelli, V. Patera, A. Schiavi, A. Sciubba, G. Traini*

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.

No established technique capable of providing the required accuracy on the dose release exists for carbon beam PT monitoring. Since 2012 [1-2], an experimental campaign was started to precisely characterise the production of secondary particles during the treatment and in particular charged fragments emitted at large angles. In the following years [3-4] we have demonstrated that charged fragments are abundantly produced in PT treatments using He, C and O ions as projectile and that a correlation between the fragments production spectrum and the dose release shape can be obtained.

In order to exploit the detection of secondary charged fragments (mainly protons) [5], a novel detector, the 'Dose Profiler' (DP) has been designed, developed and built in the SBAI department laboratory and workshop [6-8]. The research work has been funded by different institutions (MIUR: INSIDE prin project, Museo Storico della Fisica e Centro Studi e Ricerche Enrico Fermi, and the Istituto Nazionale di Fisica Nucleare) and has been carried out mainly at the SBAI department. The design and development phase, carried out in 2015–2017, ended in May 2017 with the detector construction and assembly in the SBAI workshop as shown in Fig. 1.

The protons are detected in the DP using 16 subsequent layers of plastic scintillating squared fibres (500  $\mu\text{m}^2$  area) arranged in pairs of planes in which the fibres are arranged along the vertical and horizontal axis, providing a three dimensional point, for each pair of planes and a total of 8 measure points for a proton track traveling inside the full detector. A total of  $\sim 3000$  readout electronic channels are used to readout the full detector whose active volume is  $\sim 20 \times 20 \times 16 \text{ cm}^3$ . The detection technology provides a small cost solution to achieve a very high detection efficiency (larger than 90%) over a large volume, with the needed backtracking resolution ( $\sim 8 \text{ mm}$  single track resolution is obtained at  $\sim 50 \text{ cm}$  from the target).

The detector performances have been benchmarked using proton and carbon ion beams in the Trento APSS

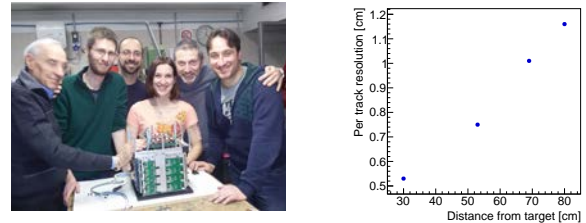


Figure 1: (Left) Final assembly of the DP detector, carried out in the SBAI department workshop of the “La Sapienza” University. The ‘naked’ detector is shown, with the readout boards (in green) and the aluminum inserts used to cool the readout circuits. (Right) Back tracking resolution obtained at different distances from the target.

and Pavia CNAO facilities. The DP was operated smoothly in clinical operation conditions (incoming particle rates larger than 100 kHz and a total readout dead time in the 3–5  $\mu\text{s}$  range) with performances that matched the design values. Different targets have been used for the performance assessment: a small plastic sphere was used to evaluate the tracking resolution while an antropomorphic phantom was used to evaluate the detector performance in treatment like conditions. The results have been presented in several key international conferences in the field [M. Marafini, RAD2015 Montenegro (2015); A. Sarti, SRHITS2015 Osaka (2015) and ICTRPHE2016 CERN-Geneva (2016); S. Muraro, VCI Vienna (2016); I. Mattei, MEDAMI Orosei (2017); G. Traini, ICNTRM Strasburgo (2017)].

Starting from 2018 the DP will be used in the CNAO centre, within the INSIDE2 project, for carbon ion treatment monitoring of selected patients allowing to assess the final accuracy achievable in clinical applications.

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## P-5. FragmentatiOn Of Target (FOOT) studies

V. Patera, M. Magi, M. Marafini, R. Mirabelli, A. Sarti, A. Schiavi, A. Sciubba, G. Traini

In the last decade a continuous increase in the number of cancer patients treated with Charged Particle Therapy (CPT) has been registered, due to its effectiveness in the treatment of deep-seated solid tumors. The main advantage of this approach derives from the depth-dose profile of charged particles, where the maximum of the dose is deposited at the range end (Bragg Peak, BP) usually seated on the cancer region, allowing to spare healthy tissues. Furthermore the increase in Linear Energy Transfer (LET) in the BP region produces an enhanced biological effectiveness in cell killing, as compared to conventional photon radiation, that can be quantified using the Relative Biological Effectiveness (RBE). In proton treatment a constant RBE value equal to 1.1 is currently assigned to protons in clinical practice. However, radiobiological measurements show a significant increase in RBE above 1.1 and the topic of RBE variability in protontherapy is being widely debated in recent years as using a constant RBE = 1.1 can lead to an underestimate of the dose in the healthy tissue region.

Particles produced in target fragmentation could be one of the causes contributing to the increase of proton RBE. When crossing the patient, nuclear interactions occur between the beam and the patient tissues generating a spectrum of low energy heavy recoils that depends on beam energy and target materials. These secondary charged particles have short range (e.g. order of  $10\div 100\ \mu\text{m}$ ), very high LET and then high RBE. The process of target fragmentation, which is the only relevant process of this kind in proton therapy, so far has been almost completely neglected. The new experiment FOOT (FragmentatiOn Of Target) has therefore been proposed by a large international cooperation (Universities of Bologna, Milano, Napoli, Perugia, Pisa, Roma, Strasbourg and Turin, CNAO, GSI, INFN)

The main experimental difficulty in the measurement of the target fragmentation induced by proton beams is due to the short range. An inverse kinematic approach can be pursued, studying the fragmentation of different ions beams (C, O, Ca, etc.) onto hydrogen enriched target, such as  $\text{CH}_2$  exploiting the fragments boosted energy and longer range. The H cross section is measured by subtraction from the coupled data obtained using both  $\text{CH}_2$  and pure C targets. The final goal of the experiment would be to measure the heavy fragment ( $Z>2$ ) cross section with maximum uncertainty of 5% and the fragment energy spectrum (in the “patient” reference frame) with an energy resolution of the order of 1-2 MeV/u, in order to contribute to a better radiobiological characterization of protons. Since 2015 a research effort has been devoted, within SBAI, to the experimental apparatus design aiming to reach the aforementioned sensitivity on the cross section measurements. Montecarlo calculations based on

the FLUKA code have been performed and predict that the heavier fragments ( $Z>2$ ) are forward peaked within a polar angle of  $\simeq 10^\circ$  and with a kinetic energy per nucleon peaked around the corresponding value of the primary beam.

The results of the simulation and MC analysis studies have been reported in the FOOT Conceptual Design Report [1]. The FOOT experiment was approved, and funded, by the INFN in 2017. The experimental apparatus (2 m long), developed and designed with a large contribution from SBAI and in particular of the mechanical workshop under the supervision of M. Magi, is shown in Fig. 1. The direct SBAI researchers contribution is related to the following items: the experiment and collaboration coordination (V. Patera is the collaboration spokesman), the Start Counter construction and operation (currently being performed by A. Sciubba) as well as the interaction region construction and detector integration, the reconstruction software coordination and development (being performed by A. Sarti).

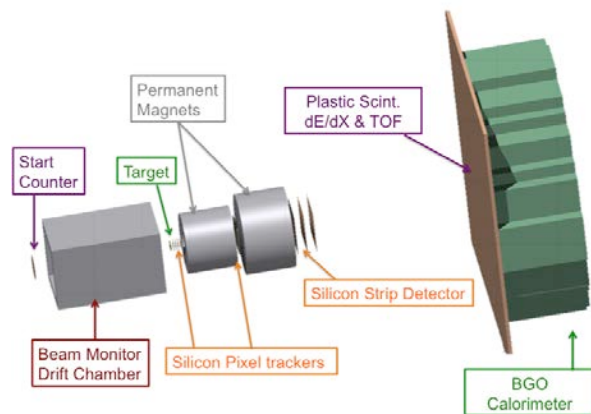


Figure 1: Schematic view of the FOOT apparatus.

The results obtained in the detector design and development phase have been presented in several key national and international conferences in the field [E. Verdolino, SIF Padova (2016); S. M. Valle, SIF Padova (2016); G. Battistoni, International Winter Meeting on Nuclear Physics, Bormio (2017); R. Mirabelli, SIF Trento (2017); S. M. Valle, MCMA Napoli (2017)].

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## P-6. Fast dose recalculation on GPU for particle therapy applications

*A. Schiavi, V. Patera, M. Senzacqua, S. Pioli, A. Mazzini*

Proton therapy has rapidly grown in the past thirty years and it has become a superior alternative to conventional radiotherapy for certain clinical indications. Proton therapy offers high dose selectivity due to the protons distinct depth dose profile which potentially allows to deliver high dose to the tumor while sparing healthy surrounding tissue. Monte Carlo (MC) simulations, which take explicitly into account all the details in the interaction of particles with human tissues, are considered to be the most reliable tool to reproduce the complexity of mixed field irradiation in a non-homogeneous environment. The advent of general-purpose programming GPU cards prompted the development of trimmed-down MC-based dose engines, which can significantly reduce the plan recalculation time with respect to standard MC codes on CPU hardware. At SBAI Department - Sapienza University we developed a novel transport code[1,2], named FRED, 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. Both, primary and secondary particles, are tracked and their energy deposition is scored along the trajectory. Effective models for particle-medium interaction have been implemented balancing accuracy in dose deposition with computational cost. At present the most refined module is the transport of proton beams in water: single pencil beam dose-depth distributions obtained with FRED agree with those produced by standard MC codes within 1–2% of the Bragg peak in the therapeutic energy range (see Fig. 1). Comparison with measurements taken at CNAO treatment center (Pavia, Italy) shows that the lateral dose tails are reproduced within 2% in the Field Size Factor test up to 20 cm. 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 (Fig. 2) at 1% of total particles in just a few minutes.

We also introduced recently in FRED the possibility of tracking carbon ions. These light ions are well suited to particle therapy applications, thanks to their high radiobiological effectiveness (RBE) when compared to standard X-rays or even proton therapy. Carbon ions in the therapeutic energy range (several hundreds of MeV per nucleon) undergo nuclear fragmentation with high probability when interacting with the human tissues. An accurate description of the dose delivered to tumor target volume and the surrounding healthy tissue demands for a refined model of Carbon nuclear fragmentation. Nuclear fragments are lighter than the primary Carbon ion, and, having typically the same kinetic energy per nucleon, travel to high depth in the patient, delivering a significant amount of dose outside the desired target

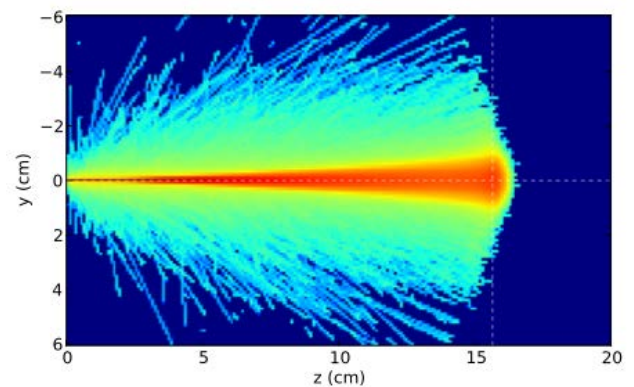


Figure 1: Dose map of a monoenergetic beam of protons in liquid water reproduced with FRED .

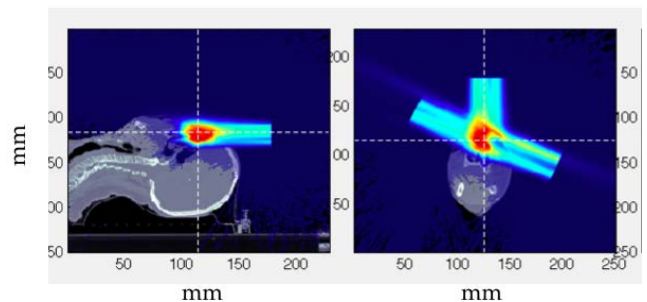


Figure 2: Patient plan recalculation for 3 separate proton fields (sagittal and transverse planes).

volume. Theoretical models and their implementation in standard MC codes do not agree very well with measured data in this interaction regime. In particular fragment multiplicity, angular and energy distributions differ significantly from model to model. New data are needed in order to improve the accuracy of dose calculation with numerical tools, and our group is committed to several activities and experiments which will supply new sets of Carbon fragmentation data in the next few years. In preparation, we added in FRED the capability of importing double-differential cross section tables for Carbon fragments distributions. A simple scaling model in energy has been developed, and successfully tested on data obtained at GANIL and CATANA experiments.

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## P-7. MONDO (MONitor for Neutron Dose in hadrOntherapy)

*M. Marafini, M. De Simoni, M. Fischetti, R. Mirabelli, V. Patera, A. Sarti, A. Schiavi, A. Sciubba, G. Traini, S. M. Valle*

Tumour control is performed, in Particle Therapy, using particles and ions whose high irradiation precision enhance the treatment effectiveness while sparing the healthy tissues surrounding the target volume. Since neutrons can release a significant dose far away from the tumour region, as shown in Fig. 1(Left), precise measurements of their flux, production energy and angle distributions are eagerly needed in order to improve the Treatment Planning Systems software, so to predict not only the normal tissue toxicity in the target region, but also the risk of late complications in the whole body. An experimental effort devoted to the precise characterisation of the neutron production is required. The technical challenges posed by a neutron detector aiming for a high detection efficiency and good backtracking precision are addressed within MONDO [1,2], a project developed at Museo Storico della Fisica e Centro Studi e Ricerche E. Fermi (CF) with a SIR project (MIUR) and G5 INFN fundings and with the partnership of SBAI department.

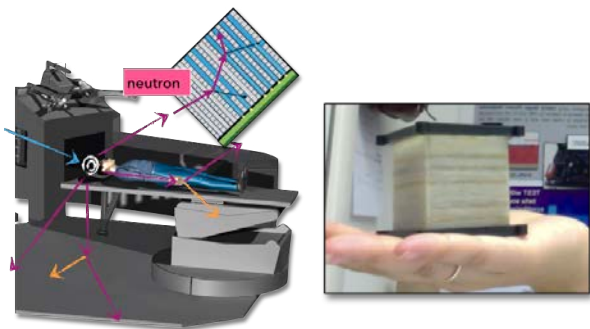


Figure 1: Left. Schematic representation of the secondary neutrons produced in PT interacting in the treatment room. The MONDO detector is shown on top of the scratch. Right. First MONDO prototype.

The MONDO project aims at the development of a compact, high-resolution tracking detector tailored for the characterisation of the secondary ultra-fast neutron production in PT treatments (energy range [20-400MeV]). Within MONDO the chosen tracker technology will be based on layers of scintillating fibres used as an active target for the neutron detection. One of the main interaction mechanisms of ultrafast neutrons in scintillators are the elastic scattering with hydrogen nuclei. In the events in which the neutron undergo a double elastic scattering (DES), if both proton recoils are measured, the neutron energy and direction can be reconstructed, allowing the measurements of the neutron energy and angular distribution.

The final detector will be a matrix of  $10 \times 10 \times 20 \text{ cm}^3$  (layers of squared scintillating fibres,  $250\mu\text{m}$ ). A dedi-

cated innovative new silicon sensor based on SPAD (Single Photon Avalanche Diode) array technology, SBAM, is under development in collaboration with the Fondazione Bruno Kessler (FBK) [3]. A small prototype of neutron tracker ( $4 \times 4 \times 4.8 \text{ cm}^3$ ), shown in Fig. 1 (Right), has been built in the mechanical workshop of SBAI. The device has been tested with cosmics, electrons and therapeutic protons at TIFPA/ASSP Trento. The number of expected interactions in the detector, obtained using a MC simulation, is shown in Fig.2.

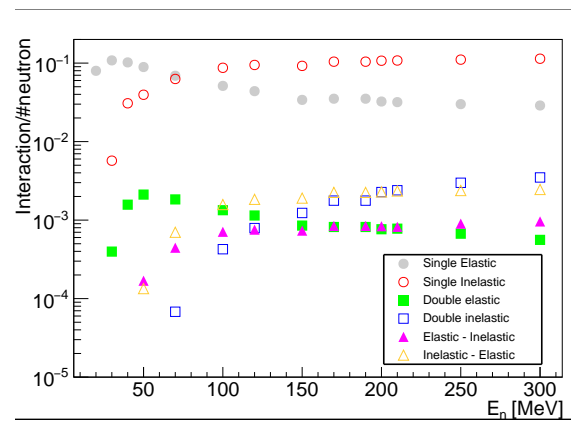


Figure 2: Number of interactions per primary neutron as a function of the neutrons initial kinetic energy.

Single elastic scattering interactions (grey, full circles) are dominant below  $100 \text{ MeV}$ , while inelastic scattering interactions (red, open circles) are dominant for higher energies. Consequently, DES interactions (green, full squares) are dominant for lower energy neutrons. Above  $120 \text{ MeV}$ , mixed interactions (yellow, open and purple, full triangles) and double inelastic scattering interactions (blue, open squares) make an important contribution in the background noise.

The MONDO detector is under construction at SBAI and the SBAM sensor first chip (FBK-CF) will be available for the end of the year. The results have been presented in several key international conferences in the field [M. Marafini, SRHITS2015 Osaka (2015), and AT-TRACT Barcellona (2016); R. Mirabelli, SIF Padova (2016); G. Traini, iWorld Cracovia (2016); I. Mattei, SCINT Chamonix (2017)].

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## P-8. New Organic Scintillators

*L. Mattiello, V. Patera, A. Sciubba, M. Marafini, A. Belardini*

Organic scintillators are broadly classed into three types, crystalline, liquid, and plastic, all of which utilize the ionization produced by charged particles to generate optical photons, usually in the blue to green wavelength regions. Plastic scintillators are by far the most widely used while liquid organic scintillator is finding increased use. Plastic scintillator densities range from 1.03 to 1.20 g cm<sup>3</sup>. Typical photon yields are about 1 photon per 100 eV of energy deposit. A one-cm-thick scintillator traversed by a minimum-ionizing particle will therefore yield  $\sim 2 \times 10^4$  photons. The resulting photoelectron signal will depend on the collection and transport efficiency of the optical package and the quantum efficiency of the photodetector. The high light yield and fast response time allow the possibility of sub-ns timing resolution. The fraction of light emitted during the decay tail can depend on the exciting particle. This allows pulse shape discrimination as a technique to carry out particle identification. Because of the hydrogen content (carbon to hydrogen ratio  $\sim 1$ ) plastic scintillator is sensitive to proton recoils from neutrons. Ease of fabrication into desired shapes and low cost has made plastic scintillator a common detector element. In the form of scintillating fiber it has found widespread use in tracking and calorimetry.



Figure 1: Plastic scintillator samples, under daylight and UV light (365 nm) illumination.

The research and development efforts devoted to the seek of higher light yield, and hence an improved time resolution, are pursuing different approaches. A possibility would be to produce new aromatic compounds capable of yielding more photons per released energy: an effort in this direction started within the SBAI department with the synergy of the Chemistry and Physics applied research lines.

New aromatic compounds have been synthesized, see Fig. 1, and completely characterized from the physicochemical, electrochemical and optical point of view. In addition, scintillation measurements have been performed by means of cosmic rays, since the intended use for these new compounds falls in the field of organic scintillators, i.e., substances capable of detecting the passage

of ionizing radiation. The experimental apparatus used for that characterization is shown in Fig. 2.



Figure 2: Scintillation counting apparatus.

These aromatic compounds have a relative light yield higher than organic scintillators currently on the market, moreover, given the particular molecular structure of these compounds, they can be homogeneously dispersed at high concentrations in polymeric matrices, a necessary condition for producing scintillating samples of different shapes and sizes with a high light output. A patent application on these new organic scintillators is under development. All the applications that require the detection of ionizing radiation, and in particular all sectors that require the use and/or presence of radioactive materials, are of potential interest: medical imaging (microsurgery probes, PET, CT, radiology, etc ...), detection of radioactive particles (environmental contamination, customs controls, etc ...). Potential stakeholders interested in the invention could be international producers of organic scintillators, among them, for example, Saint-Gobain (France) ([www.crystals.saint-gobain.com](http://www.crystals.saint-gobain.com)) and Eljen Technology (USA) ([eljentechnology.com](http://eljentechnology.com)). The authors possess an excellent expertise and a vast patent production in the fields of the synthesis of compounds for Organic Electronics [1] and of particle physics [2-4].

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## P-9. Biomedical ultrasonics

A. Bettucci, M. Germano, A. Alippi

Lipid-coated microbubbles (mean diameter from  $\simeq 2$  to  $\simeq 5 \mu\text{m}$ ) 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 ( $> 10 \text{ MHz}$ ); consequently, a new generation of UCAs is being studied made of liquid solutions of nanobubbles (mean diameter  $\simeq 100 \text{ nm}$ ). 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.

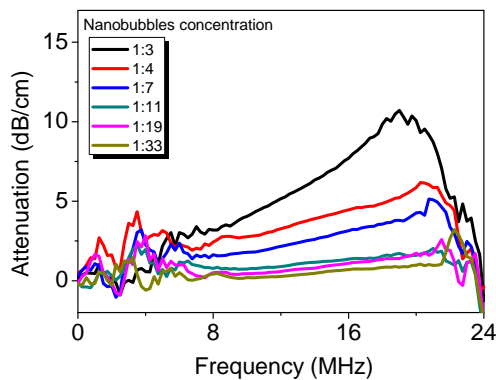


Figure 1: Acoustic attenuation spectra of lipid-coated nanobubbles as function of nanobubbles concentration

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 Rome, 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.

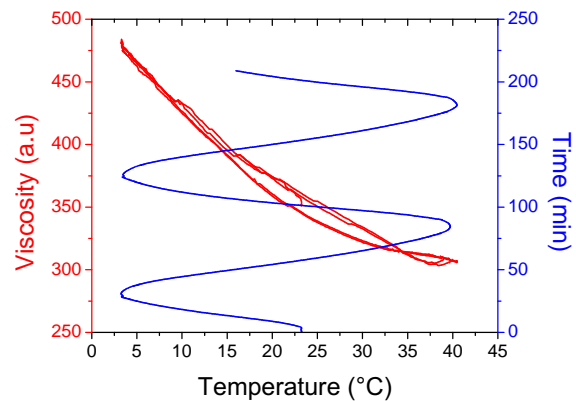


Figure 2: Viscosity of red blood cells measured through QCM-based biosensor as function of periodically varying temperature

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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## P-10. Elastic guided waves

*M. Germano, A. Alippi, A. Bettucci*

Elastic waves have several applications in very different fields such as, for example, ultrasound in medical diagnosis and treatment, non destructive testing, ultrasound-based navigation system, industrial control systems, power ultrasound in food processing, sonochemistry, ultrasound welding processes and they are used in material science for elastic media characterization, as well. In our research guided elastic waves, such as surface acoustic waves (Rayleigh waves) and plate normal modes (Lamb waves) are used to simulate some phenomena common to other wave-like fields. The main topics of our research are:

**Tunnel effect.** A forbidden propagation zone in an acoustic waveguide, created by varying the waveguide cross section, represents a potential barrier for an elastic wave packet, so that a typical quantum phenomenon like the tunnel effect, can be reproduced studying the propagation of an elastic wave into an acoustic waveguide. In particular, backward propagating Lamb waves in which the direction of the group velocity is antiparallel to the phase velocity direction, have been used to experimentally investigate the so called tunneling time through a potential barrier, where no real propagation vector is allowed. The effect of strong distortion of the tunneling wave packet and the consequent lack of causal relation between ingoing and outgoing signals from the forbidden propagation zone is avoided just for the peculiar characteristics of backward propagating waves. The almost complete analogy of the acoustic case with the electromagnetic one favors the interpretation of superluminal propagation of light pulses, giving a contribute to a still very debated topic.

**Self interference.** Near and far field vibration amplitude distribution of a particular  $S_1$  Lamb mode, generated on a steel plate by means of a wedge transducer, has been investigated. It has been found an oscillating behavior of the radial profile of the acoustic wave amplitude. This phenomenon has been interpreted and modelled as due to the interference between forward and backward propagating components of the Lamb mode, simultaneously generated at transducer/plate interface.

**Anomalous reflection and refraction.** Mode conversion is an important feature of wave propagation properly used in ultrasonic nondestructive testing through Lamb guided waves. When a wave packet with a given central frequency, and a correspondent central wavenumber, impinges on the free end of a plate, the reflected wave is a composition of the all possible normal modes compatible with the given frequency. Under

particular conditions, only one mode is reflected having a different central wavenumber with respect to the incident one. In such a case, according to the Snell's law, the reflection angle and the incident are not equal. We have also observed a special case of mode conversion where a forward propagating  $S_1$  Lamb mode is converted into a backward propagating  $S_1$  Lamb mode. In this case the reflected angle lays on the same half plane with respect to the normal direction similar to the incidence angle. This phenomenon is named negative reflection and the so-called *perfect lens* relies on it.

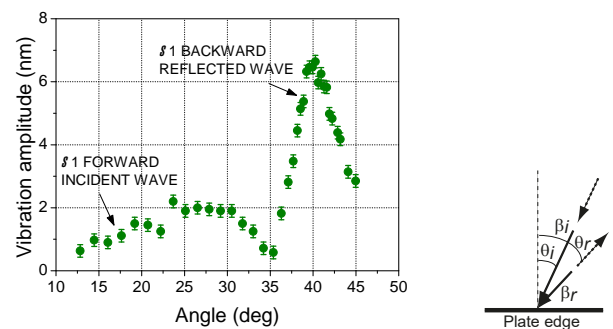


Figure 1: Profiles of the surface vibration amplitudes along a line parallel to the plate edge. On the right side, diagrams of the relative geometrical relationships: the solid vectors refer to wave vectors, the broken ones to energy propagation directions.  $S_1$  Lamb forward mode incident on the plate edge at an angle  $\theta_i = +25^\circ$  is converted into  $S_1$  Lamb backward mode and reflected at angle  $\theta_r = +35 \pm 2^\circ$ . Conversion from forward to backward mode causes the angle of reflection to be changed from the incident one and lying on the same side with respect to the normal (negative reflection).

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## P-11. Laser-driven inertial confinement fusion and high energy density plasma physics

*S. Atzeni, A. Schiavi, L. Antonelli, A. Marocchino*

In inertial confinement fusion (ICF), a cryogenic deuterium-tritium (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. Activities on ICF and more generally, on high energy density (plasma) physics (HEDP) were boosted by the demonstration of hot spot self-heating due to fusion yield by DT reactions, at the U.S. NIF laser facility [Hurricane et. al, Nature, 506, 343(2014)]. A perspective on laser fusion research was presented in Ref. 1.

In 2015-2017 SBAI plasma physics group participated in a number of projects in the fields of ICF and HEDP. Most of them were performed in the frame of a PRIN project (led by our group) and a Eurofusion project (led by a group from the University of Bordeaux), both on the ICF scheme of Shock Ignition. A few experiments were supported by the EU LaserLab programme. The main activities can be summarized as follows

**Shock ignition target studies.** In shock ignition, 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. According to earlier computations and preliminary experiments, shock ignition is highly promising, however target robustness is to be assessed. Using a metric for robustness (ITF, ignition threshold factor), we have improved target design by systematic 1D simulations. Using 2D radiation-hydro-nuclear simulations with our DUED code, we have then studied sensitivity to long-scale irradiation non uniformities and target positioning errors (Fig. 1). Simulations show that targets with larger ITF can withstand larger perturbations [2].

**Experiments on laser-plasma interaction and laser-induced shock-waves** We have participated in a number of experiments, concerning laser-driven shock waves, laser-plasma instabilities and thin target implosions. We proved the feasibility and discussed the interpretation of pulsed X-ray radiography of shocked targets [3]; the relevant experiment had been performed at Laboratoire LULI, Ecole Polytechnique. In another experiment (designed and led by one of us) and performed at LULI, we showed the importance of nonlocal conduction effects in the development of blast waves [4]. Furthermore, our DUED simulations were instrumental in the analysis of shock-driven implosions (performed at the Univ. of Rochester, by a collaboration led by an MIT group). This work provided the first evidence for kinetic effects in imploded plasmas [5].

**Synthetic diagnostics** The interpretation of ICF and HEDP experiments rely heavily on 2D and 3D simulations. Code main output consists of sequences of maps

of fluid and thermodynamic variables, which are not easily compared with experimental observables. More direct comparison requires the development of simulated, or synthetic, diagnostics, using the detailed plasma information available in the fluid simulations. This has motivated the development of simulated diagnostics coupled with DUED: i) x-ray radiography [3] for shock compression of matter; ii) neutron spectrometry; ii) fast charged particle spectrometry for stopping power measurements (in collaboration with LULI-Ecole Polytechnique).

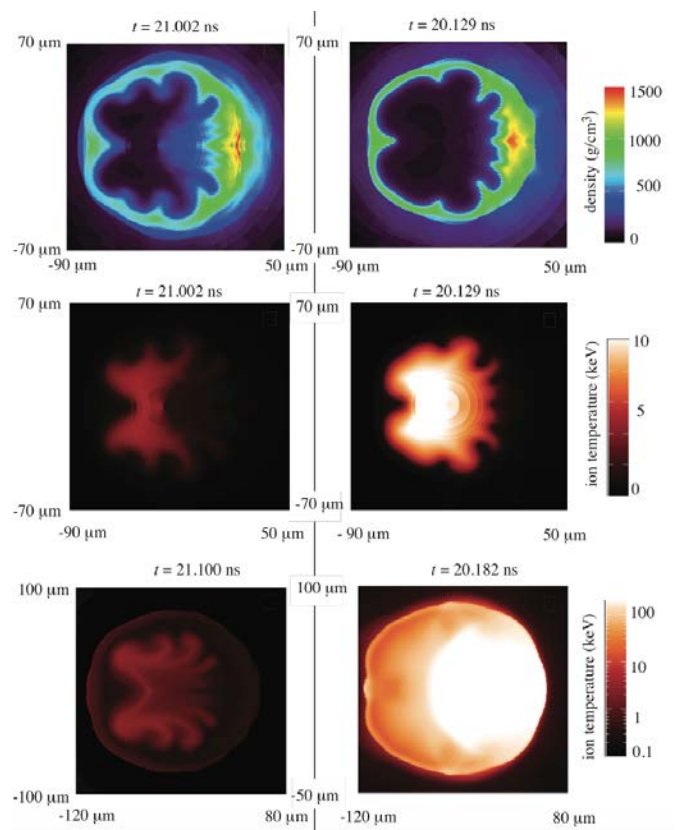


Figure 1: Simulation of shock ignition targets, driven by nonuniform laser pulses, and mispositioned. Maps of density and ion temperatures at implosion stagnation and ignition. Two targets (right and left column, respectively) are considered. Only the target with larger ITF (on the right) ignites.

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## P-12. Kinetic and hybrid simulations of plasma-based accelerators and plasma lenses

*A. Marocchino, S. Atzeni, E. Brentegani, F. Massimo, F. Mira, A. Schiavi*

Electron Plasma Wakefield Acceleration (PWBA) accelerates a bunch of electrons (witness beam) through the electric field induced in the plasma wake of a higher charge particle beam (a driver) in a plasma. PWBA can achieve accelerating gradients at least two orders of magnitude larger than conventional radiofrequency accelerators, limited by electric breakdown.

SBAI plasma group initiated a computational and theoretical activity on electron PWFA in the frame of the activities of INFN-LNF SPARC\_Lab, in collaboration with researchers from INFN-Bologna and Milano.

Accurate studies are performed with the kinetic Particle-in-Cell (PIC) code Aladyn. GAPS contributed to the upgrade of the code, originally developed by the Bologna group. Objectives of our investigations are definition of the parameters for PWFA experiments at SPARC\_Lab, as well as for future larger facilities, as investigated by the EUPRAXIA project. An example of simulation is shown in Fig. 1.

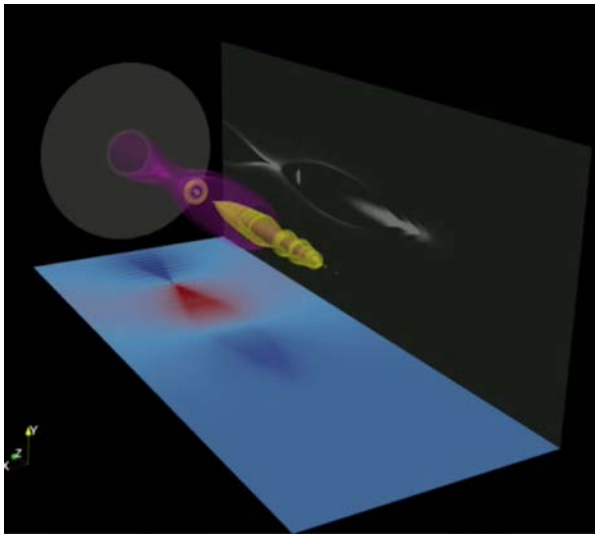


Figure 1: A 3D Aladyn simulation of PWFA. The figure shows a 3D view of plasma density, as well as density map on an axial vertical plane (vertical panel) and longitudinal E-field map on an axial horizontal plane (horizontal plane).

3D PIC simulations are the state-of-the-art tool for plasma acceleration studies. However, they require very large computing resources. To overcome such limitations, we have developed a new code, Architect, employing a 2D hybrid scheme [1]. The bulk plasma is dealt with as a relativistic fluid, while the electron bunches are described by a kinetic model. Detailed tests (see, e.g. Fig. 2) have shown that this new approach can properly simulate PWBA schemes up to a weakly nonlinear acceleration regime [2]. Thanks to the modest computing

times Architect can be used for design and sensitivity studies, requiring large number of runs.

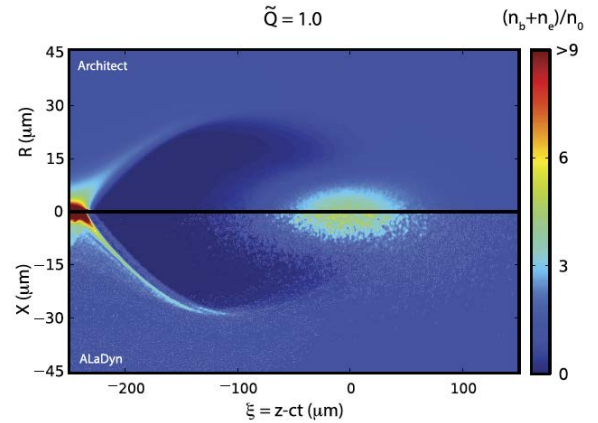


Figure 2: Cylindrical plasma channel for PWBA. A bunch is moving from left to right. The green-yellow spot on the axis around  $\xi = 0$  is the driver bunch; on its left we observe a depleted *bubble*. The figure shows maps of electron density computed with the hybrid code Architect (top panel) and fully kinetic PIC code Aladyn (bottom panel) in a weakly nonlinear regime, confirming the adequacy of the much faster hybrid code.

Thin cylindrical plasmas, contained in a capillary, and heated by an electrical discharge, can be used as lenses for particle beams. Focusing is caused by the magnetic field generated by the axial plasma current. To contribute to SPARC\_Lab activities on plasma lenses, we first simulate the plasma discharge by a properly upgraded version of the GAPS plasma-hydrodynamics DUED code. We then use the obtained distributions of plasma density and magnetic field as input to Architect simulations of beam propagation inside the capillary. Preliminary results have been published in Ref. [3].

This work was performed in collaboration with E. Chiodroni and A. Ferrario (LNF-INFN) and A. R. Rossi (INFN Milano).

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## P-13. Laser-Accelerated Proton Beams as Diagnostics for Cultural Heritage

*M. Scisciò, P. Antici*

In the last few decades, a large effort has been put into applying innovative Physics and Chemistry research techniques for diagnostic and conservations of objects of interest for Cultural Heritage (CH). The complete chemistry of the bulk material can be retrieved using sophisticated (and expensive) nuclear physics techniques such as Proton Induced X-ray and Gamma Emission (PIXE and PIGE) [1]. The conventionally accelerated proton beams that are currently used for implementing these techniques, can be replaced by laser-accelerated protons, as generated by interaction of a high-power short-pulse laser with a solid target, potentially allowing more compact and less expensive facilities.

The configuration of the laser-driven PIXE is similar to a typical PIXE setup, with the only difference that the conventional ion source is replaced with a laser-based one (see Fig. 1): The high-power laser is impinging a commercially available solid target which acts as proton source. The laser-generated protons are used to irradiate a CH sample: The X-rays, produced in the interaction between the laser-generated protons and the sample to be probed, can be detected by an X-ray detector that implements a diffraction crystal and radiation-sensitive image plates (IP).

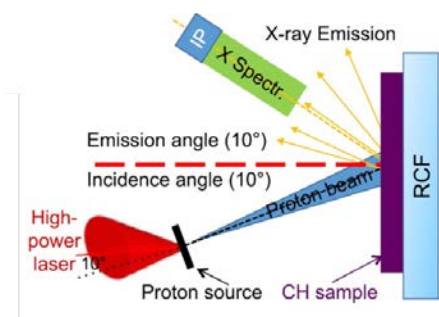


Figure 1: Experimental setup of laser-driven PIXE.

The experiments have been performed on the TITAN laser of the Jupiter Laser facility (LLNL, USA), producing laser pulses of about 220 J in 700 fs and operating at a wavelength of 1.054  $\mu\text{m}$ . The laser beam, focused down to about 9  $\mu\text{m}$  focal spot diameter (FWHM) - producing an on-target intensity  $I \approx 10^{20} \text{ W/cm}^2$ , was used for interacting with a commercially available Gold target (10  $\mu\text{m}$  thickness) in order to accelerate protons in the laser-forward direction using the TNSA (target normal sheath acceleration) mechanism [2]. The laser-generated protons (with a broad, exponentially decreasing spectrum extending up to 30 MeV) impinged the CH sample with an incidence angle of 10°. As samples we used pure silver (97%, thickness 200  $\mu\text{m}$ , impurities of Cr, Ti and

Cu). The results of a single-shot PIXE conducted on silver are indicated in Fig. 2.

As visible from the RCF positioned behind the sample (Fig. 2A), the silver target was fully covered by the proton beam, i.e. the protons irradiate a surface of several . The IP of the PIXE spectrometer (Fig. 2B) shows three well-defined bands corresponding to the Ag K (first order) and L (second order) bands, as evaluated from the Bragg law.

The Gaussian-convoluted spectrum (obtained using the cross sections for each line) is shown in Fig. 2C. The leftmost line, close to the zero-order (the intense round spot in Fig. 2B), corresponds to the first order K-alpha line (22.2 keV) while the two adjacent lines on the right side can be attributed K-beta lines of Ti and Cr respectively (4.93 and 5.94 keV). The one-shot PIXE data are in perfect agreement with those obtained by conventional XRF on the same sample (inset in Fig. 2C), which indicate the presence of the L-alpha line of Silver (3 keV) and K-beta lines of Ti and Cr. The obtained results confirm the feasibility of laser-driven PIXE, which can be performed in a single laser shot [3].

This work was performed in collaboration with M. Barberio, S. Veltri (INRS-Quebec) and A. Morabito (INFN).

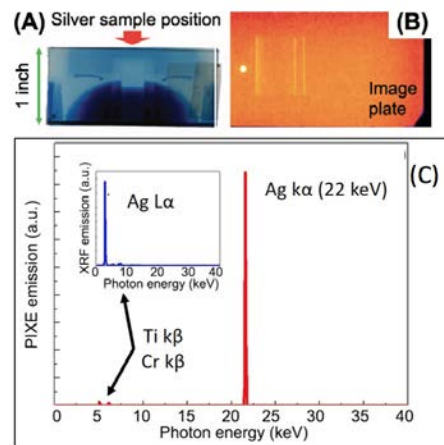


Figure 2: (A) Silver sample mounted on an RCF. (B) IP detecting the emitted X-rays. (C) Retrieved PIXE spectrum and RXF analysis (as reference) of the Ag sample.

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## P-14. Laser physics for particle accelerators and radiation sources

*M. Petrarca, A. Curcio, V. Dolci*

In our group, we follow two main lines of research that are based on the use of the electromagnetic radiation (e.m.) as a diagnostic or as a driver to monitor or excite a particular system. Most of the studies are devoted to applied physics for particle accelerators or the environment, in particular laser wakefield acceleration and electron bunch diagnostics for the first topic, lightning control and radiation sources for the second.

Novel acceleration schemes include particle acceleration driven by intense pulses of e.m. radiation generated by lasers and propagating in plasma, where they induce a strong longitudinal electric field, called a 'wakefield', which can be used to accelerate charged particles. This technique is called Laser Wakefield Acceleration (LWFA). In [1] the propagation of an intense laser pulse in a gas-filled capillary has been studied. The capillary acts as waveguide, and is required to counteract the diffracting effects that the e.m. pulse undergoes along its propagation, therefore extending the length of the accelerating section (i.e. the longitudinal region of space along which the particles are accelerated). We have studied how the capillary modes are excited and how mode excitation reflects in the wakefield, as well as the effects of the ionization of the gas on this wakefield.

The studies carried out to address issues related to materials damage and to the high laser energy ( $> 1$  J) required to generate the wakefield led to a new idea [2]. This is based on driving the wakefield belongs by Terahertz (THz) radiation rather than by Near Infrared radiation (NIR). Reference [2] is the first work in the literature to address the generation of the wakefield by a THz pulse. The proposed acceleration scheme is compared to the more standard one where NIR pulses are employed. The different scenarios of applicability of the two complementary schemes are discussed.

Electromagnetic radiation emitted by charged particles undergoing acceleration/deflection or interacting with a solid-target can be used to retrieve information on the characteristics of the particle bunch (transverse and longitudinal dimension, particle transverse divergence and energy spread) or can be used for other kinds of experiments. For example, we have demonstrated that in the  $\text{Bi}_2\text{Se}_3$  topological insulators electromagnetic-induced transparency is achieved under the application of a strong terahertz electric field [3].

Several studies on the use of betatron radiation emission in novel diagnostic schemes of practical interest for LWFA have been performed. A new single-shot, non-intercepting monitor of the transverse profile of plasma-accelerated electron beams has been presented [4]. Moreover, we have studied emission of betatron radiation during a LWFA process in gas-filled capillary, and described how emission of this radiation is affected by the capillary

modes [4].

The propagation of high-intensity laser pulses in gasses (air) is characterized by several non-linear processes (self-focusing, self-phase modulation, ionization, etc.), which give rise to the so-called 'filamentation regime' of propagation. This regime can be of practical interest for various important applications e.g. remote triggering of lightning, LIDAR, secondary emission sources, particles acceleration, etc... Several studies have been performed and reported in literature for the single filamentation regime (which is ignited by a low power laser pulses containing 1-10 mJ of energy in 50 fs temporal pulse width). The multi-filamentation regime, which is the filamentation regime started by very high power laser pulses (containing  $> 100$  mJ of energy in 50 fs temporal pulse width), is instead still under study. To examine this regime of non-linear laser pulse propagation, the physics of laser ablation by femtosecond laser pulses has been studied [5]. In particular it was shown that for optically dissimilar materials (metal, glass, semiconductor), the value of fluence transmitted into the material at the point of ablation threshold, if calculated using the linear (unperturbed by the laser field) complex index of refraction, is nearly independent of the angle of incidence and polarization. Then, by exploiting this knowledge, a novel diagnostic technique that is capable of determining the spatial distribution and properties of the multi-filamentation regime, as well as the intensity threshold carried by each filament, has been proposed. In particular, we studied the nonlinear propagation of multiterawatt femtosecond laser pulses at 800 nm wavelength in air, under different external focusing conditions [6]. For very tight focusing the propagation regime is reminiscent of the nanosecond optical breakdown, while in the case of moderately strong focusing, multiple individual filaments are formed well before the focus and propagate through the focal zone without coalescing into a single or few superfilaments.

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## P-15. Electron Microscopies and Nanoscopies (EMINA)

*M. Rossi, D. Passeri*

Since its establishment, EMINA group has been committed with the nanoscale characterization of materials using advanced microscopy methods, i.e., electron and scanning probe based microscopies.

In particular, atomic force microscopy (AFM) is routinely used for the morphological characterization of a broad range of materials, from microelectronic devices to biological samples, in the framework of different scientific collaborations in which EMINA is involved, e.g., the study of vesicular systems for drug delivery or the self-assembly of molecular structures [1].

Moreover, EMINA group's research has been focused on the development, implementation, validation, and application of advanced scanning probe microscopy (SPM) based methods for the characterization of different physical properties (e.g., mechanical, magnetic, electric) at the nanometer scale.

- Mechanical characterizations** The specific techniques for nanomechanical characterizations using AFM include contact resonance AFM (CR-AFM), AFM-based nanoindentation, HarmoniX™, and peak force quantitative nanomechanical mapping (PF-QNM™). Their synergistic and complementary use allowed us to investigate different materials, e.g., from soft polymeric films, nanofibers [2], nanocomposites, and cells (see, e.g., Fig. 1) [3] to stiff materials with gemological and mineralogical interest;
- Magnetic characterizations** As for magnetic methods, magnetic force microscopy (MFM) has been implemented to allow accurate quantitative determination of magnetic properties of materials at the nanoscale by developing an experimental approach enabling the identification and removal of nonmagnetic (electrostatic) artifacts. This advanced MFM technique allowed us to investigate magnetic nanoparticles, e.g., by acquiring magnetization curves of single isolated nanoparticles [4];
- Electric characterizations** Methods for electric characterization, i.e., electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM) have been also employed to study nanoscale systems such field emitters or silicon-carbon based nanostructured materials [5].
- Chemical characterizations** Finally, in collaboration with Lfoundry - A SMIC Company, EMINA has developed also tip-enhanced Raman spectroscopy (TERS) for the study of strain in microelectronic devices [6].

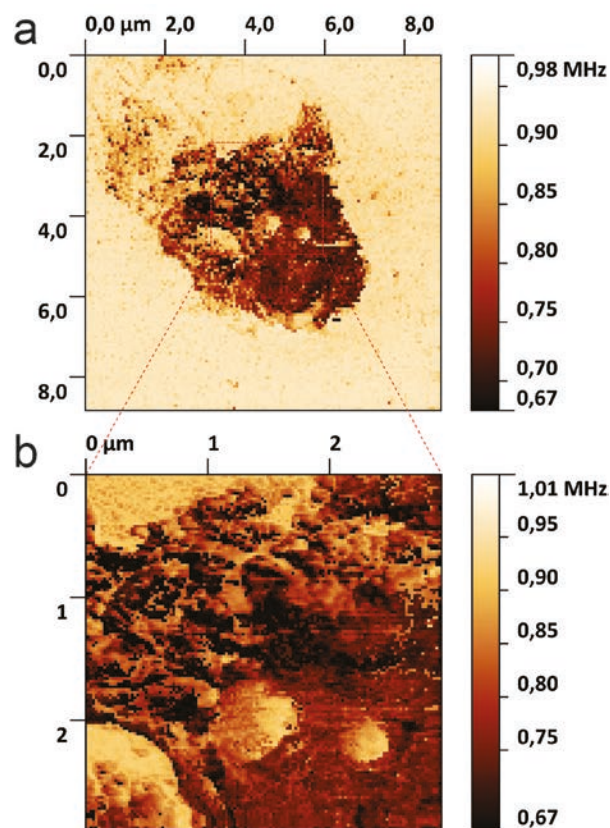


Figure 1: Mechanical mapping of a microglia cell internalizing agglomerates of magnetite nanoparticles

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<http://www.nanothings.it/eminalab/>

## P-16. Density Functional Theory and beyond: surface, bulk and optical properties of materials and nano-structures

*G. Zollo, F. Gala, L. Mattiello*

Density Functional Theory (DFT) and related techniques are powerful first-principles methods that allow the quantum mechanical study of atomistic systems with meaningful sizes concerning surface, bulk and optical properties.

**Surface physics: water self-assembling on TiO<sub>2</sub> surface** Experiments evidence that water molecules belonging to the first monolayer (ML) are mobile on the (101) anatase TiO<sub>2</sub> surface below 190 K and form clusters along the  $[11\bar{1}]/[1\bar{1}\bar{1}]$  surface directions. These

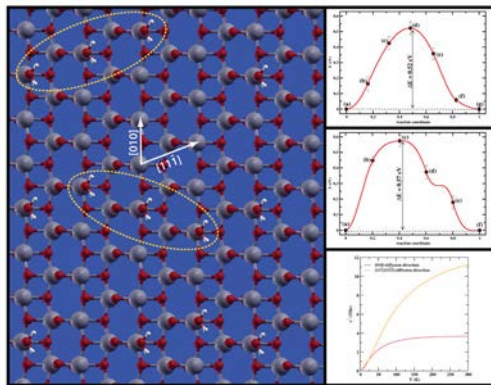


Figure 1: Water clustering onto the anatase (101) surface

dynamical processes have been understood in the context of the transition state theory with a variety of computational techniques, namely DFT, Density Functional Perturbation Theory (DFPT) and Kinetic MonteCarlo (KMC). The dynamical process of water clustering is evidenced and the characteristic time scale of self-assembling phenomena is calculated with nice accordance with the experimental evidences [1].

**Solid state physics: T<sub>c</sub> degradation in off-stoichiometry Nb<sub>3</sub>Sn superconductors.** The superconducting properties, and the related phonon mediated electrons coupling, have been studied for the A15 Nb<sub>(3-x)</sub>Sn<sub>(1+x)</sub> with varying  $x$ . A key quantity, the mass enhancement parameter that, according to the Allen-Dynes formula, determines the superconducting critical temperature, has been explicitly calculated in the context of the DFPT and the Eliashberg theory. The phonon mediated electron pairing at different compositions degrades with the Sn content and the phonon modes that are responsible of the critical temperature degradation are evidenced [2].

**Optical properties: absorption spectra of donor molecules for organic solar cells.** Many body per-

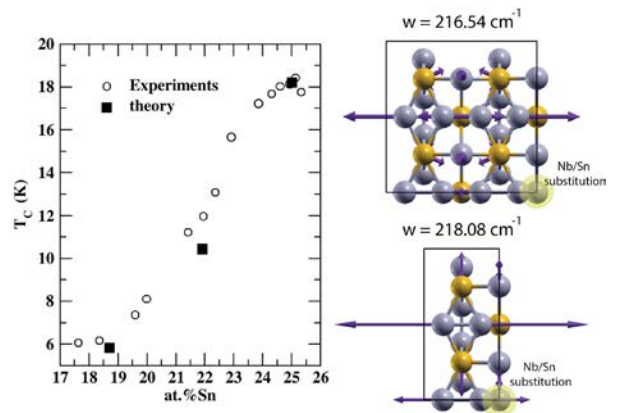


Figure 2: T<sub>c</sub> degradation of Nb<sub>(3-x)</sub>Sn<sub>(1+x)</sub> compounds and the surviving coupling phonon modes.

turbation theory (MBPT) has been employed to study the optical absorption properties of a newly synthesized oligothiophene molecule (BT2N) for solution-processed bulk-heterojunction solar cells. To this aim, the quasi-particle energies obtained by MBPT and DFT, have allowed to solve the Bethe-Salpeter equation for the excitonic Hamiltonian. The marked excitonic nature of the experimental absorption spectrum has been explained looking at the inter-molecular transitions between the  $\pi$ -stacked poly-conjugated molecules that are typically obtained in solid-state organic samples [3].

Part of the above work was performed in collaboration with L. Agosta (external collaborator) and G. De Marzi (ENEA).

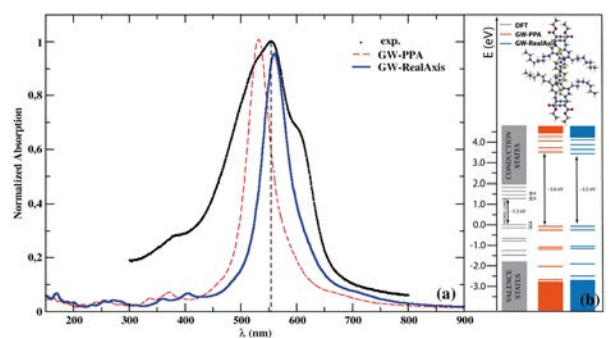


Figure 3: Theoretical and experimental BT2N absorption spectra.

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## P-17. Plasmonics and photonics : linear and nonlinear optical properties of metamaterials and metasurfaces

*C. Sibilìa, M. Centini, A. Belardini, M.C. Larciprete, R. Li Voti, G. Leahu, E. Petronjicich, G.M. Cesarini, M. Bertolotti*

One of the objectives of the groups research activity has been for some time now, to study the most efficient propagation conditions of optical fields in linear and nonlinear optical materials, in order to optically control the propagation conditions, and also to be able to generate frequencies of the e.m. field not easily obtainable with the current laser sources (uv or far infrared), and to obviate the limitations imposed by nature regarding the rather modest values of non-linear optical susceptibility and the compensation of the refractive index dispersion by means of geometry. A study was undertaken to examine the spatial localization of the e.m. field in non-homogeneous structures . Numerous effects have been studied: nonlinear frequency conversion to visible with semiconductor materials, including non classical effects [1], second harmonic generation with electro-optical materials ( A.Belardini ) and in appropriate guided geometry, such as a photonic crystal; "negative refraction" conditions with anisotropic crystals, nanostructures [2], metallic based materials (plasmonic, meta materials) for different types of applications (M.Centini ). Among the various properties studied we would like to mention the problem of modifying the infrared emission of an object, that is the so-called thermal camouflage (M.C.Larciprete). With this term we mean the variation of the emissivity of an object at a given temperature to adapt it to that of the surrounding environment, from the IR point of view. The general approach is to develop a flexible coating ( smart textiles) to be applied to the surface of the body to be screened.

and nonlinear optical properties of artificial chiral material and surfaces. The work started with the study of chiral response of chromophores (bacteriorhodopsin), and continued with the study of artificial (extrinsic) chirality of metallic meta-materials and surfaces including semiconductor nanowires. Among the optical properties, we have to mention thermo-optical and photoacoustic properties (R.Li Voti) of metasurfaces [3], an example of this is shown in the fig.1, where a GaAs Nanowire surface has been studied by means of photoacoustic techniques(PA). We would like to mention the recent activity on the study of optics and nonlinear optical properties of phase change materials. Furthermore, the collaboration with F.A.Bovino of Leonardo Company has produced a number of works and activities in the frame of quantum computing ( COPERNICO project).

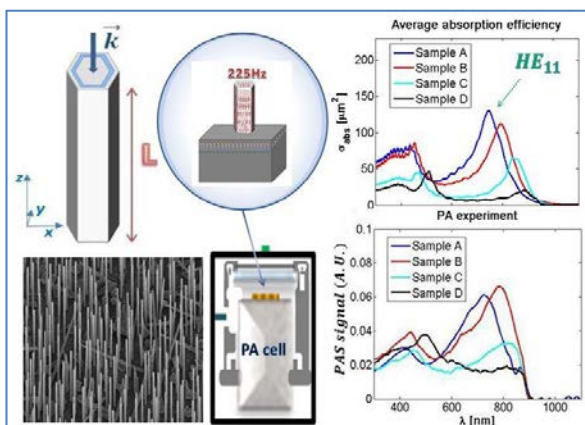


Figure 1: GaAs NW and PA measurements

A more recent research line includes both theoretical and experimental activities in an international frame of cooperation with different groups, to study the linear

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## P-18. Characterisation of nanostructures by second harmonic generation

A. Belardini, M. Centini, C. Sibilìa

Optical second harmonic generation (SHG) is a very sensitive technique to characterize the symmetry and morphology of nanopatterned surfaces. It is a background free detection technique that detects magnetic dipole or electric quadrupole contributions in the electromagnetic response of investigated media and more importantly a large signal can be produced in macroscopic media lacking inversion symmetry. By using SHG we characterise subwavelength features of self assembled nanopatterned surfaces as gold nanoantennas on polystyrene spheres, tilted gold nanowires on silicon and gold decorated GaAs nanopillars as well as metasurfaces composed by a silver and germanium. In fig.1 we show the dramatic difference of the SHG signal as a function of polarisation of light when the pump laser impinges on a 100 nm thick silver film layer (fig.1b) and on the metasurface where the silver grains are surrounded by a thin germanium coating (less than 1nm) [1].

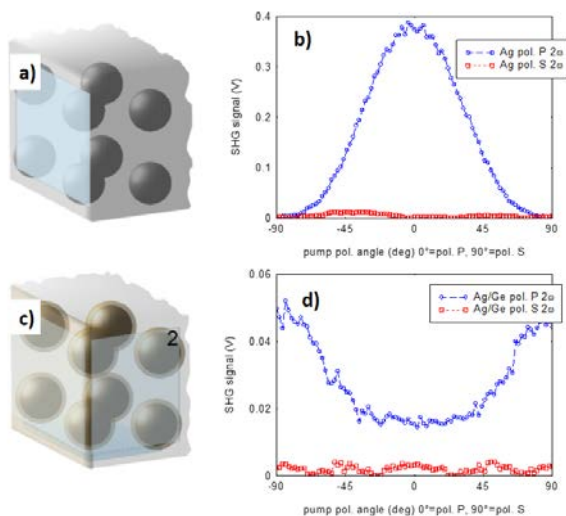


Figure 1: Figure 1: a) sketch of a polycrystalline silver film composed by crystal grains; b) SHG measurements on silver film as a function of input polarisation; c) sketch of a metasurface composed by silver grains surrounded by a Ge thin coating; d) SHG measurements on the Ag-Ge metasurface.

An important form of symmetry breaking is chirality, the lack of mirror symmetry. The characterisation of surface chirality by SHG experiments has had an enormous impact on the study of chiral molecules that are important for progress in the life-sciences and pharmaceutical industries. Among chiral symmetry, the extrinsic or pseudo-chirality is investigated for different potential applications. Extrinsic chiral (meta)surfaces

have an achiral structure, yet they can give rise to circular dichroism when the experiment itself becomes chiral. In fig.2 we show how SHG measurements can lead to the clear identification of the symmetries that are present in a self-assembled metasurface formed by tilted gold nanowires on a silicon substrate [2].

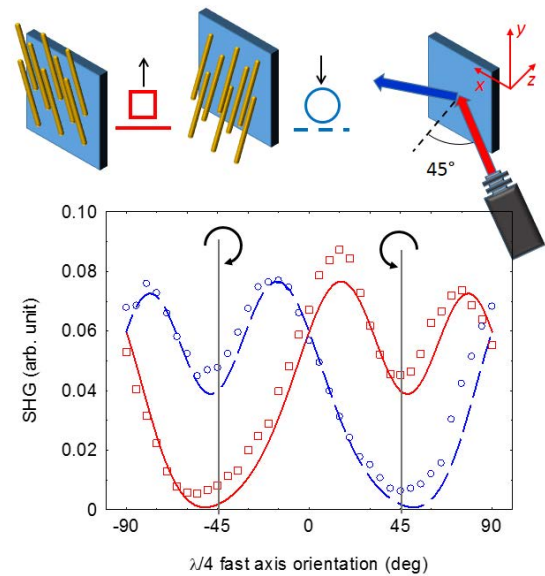


Figure 2: Figure 2: SHG measurements of the extrinsic chirality in a sample formed by gold tiled nanowires.

We put in evidence that, since the second harmonic generation process, is very sensitive to the symmetry breaking at the interfaces of investigated samples; it can be orders of magnitude more sensitive to the chiral behaviour of nanostructures with respect to analogue linear optical measurements. This shows the potential of such a technique in the field of nanotechnology characterization.

Part of the activity was performed in collaboration with the Ultrafast Photonics Lab headed by Prof. E. Fazio.

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## P-19. Multipolar nano antennas for tailored infrared thermal emission and nanoscale radiative heat transfer

*M. Centini, M.C. Larciprete, A. Belardini, R. Li Voti, C. Sibilìa*

The possibility to control the infrared absorption and thermal emission on subwavelength scales has attracted large interest in the recent years thanks to the opportunities granted by nanostructured metamaterials such as plasmonic nanoantennas. The electromagnetic properties of these systems are dominated by multipolar resonances arising from interactions and coupling between different elements. Both metallic and dielectric nanostructures, supporting electric and magnetic resonances, have been studied in order to tailor the far field emissivity of a point source (i.e. a quantum dot) as a function of the wavelength and of the position of the feeder with respect to the antenna ensemble [1].

We have recently numerically shown that a similar concept can be applied if thermal radiation from heated coupled nanoantennas is considered. We developed a numerical 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 smaller than the thermal wavelength [2]. In figure 1 we show as an example the relative emissivity for a system composed by three Au rods, detailed in reference [2]. We note that the relative emissivity spectrum exhibits both electric (a) and magnetic and electric (b) dipole resonances. The multipolar emission is responsible for the directionality of the emission pattern (b).

In order to introduce a control of the emissivity as a function of the temperature, thermochromic and phase change materials have been considered. In particular Vanadium dioxide (VO<sub>2</sub>) has become a widely-studied material for applications such as metamaterials, smart windows and super-capacitors [3]. The control mechanism is achieved by taking advantage of the metal-insulator phase transition of VO<sub>2</sub> at its critical temperature (68°C). The drastic changes of the VO<sub>2</sub> refractive index across its metal-insulator phase transition produce strong differences in the behavior of the overall system by creating or destroying evanescent wave coupling between different elements of the nanoantenna.

Finally, in order to investigate the temporal dynamics of the radiative emission modulation in the future, we are studying out of equilibrium systems. In this case a radiative heat transfer between components of the antenna array has to be taken into account in the numerical model.

The study of IR thermal nano-emitters is crucial for the realization of coherent thermal nano-sources in the mid and far IR for sensing applications and thermal management as well as thermal logic gates on the nanoscale [4]. Thus we are studying mechanisms to combine nanoscale emitters with photonic elements such as

waveguides in order to manipulate the evanescent components of emitted radiation for the creation of a new class of integrated sources.

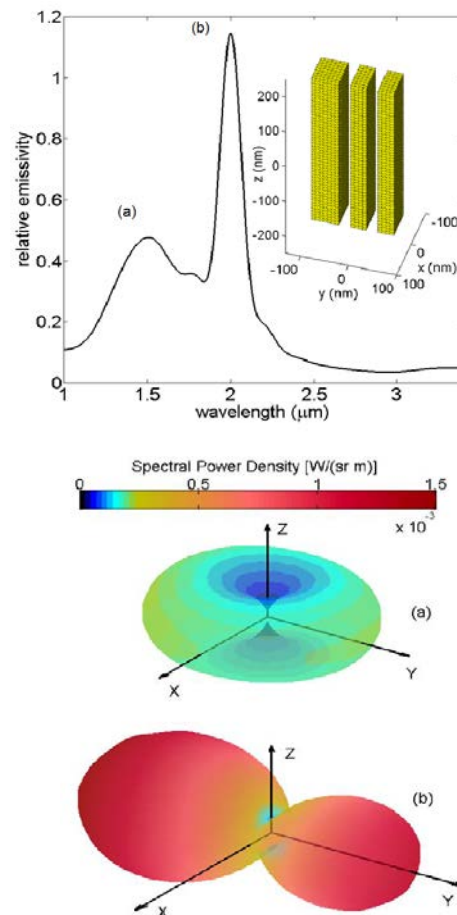


Figure 1: relative emissivity as a function of wavelength calculated for the coupled Au dipole nanoantennas sketched in the inset and described in reference [2]. The corresponding emission patterns of the two main peaks labelled (a) and (b) are depicted below.

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## P-20. Infrared radiation manipulation in polar metamaterials

*M.C. Larciprete, M. Centini, R. Li Voti, C. Sibilìa*

In recent years, much effort has been expended upon managing and tuning the radiative properties of structures and material surfaces in the infrared (IR) wavelength range (3–12 micron) for several applications, such as thermal radiation control as well as IR sensing [1].

Polar materials are particularly suitable for this purpose, i.e. those materials where it is possible to excite the collective oscillations of the lattice ions, just like the collective modes of electrons in metals. The polarization waves of the crystal lattice are called surface polaritons, similarly to the surface plasmons excitable in the ultraviolet and visible in metals. Since the oscillation frequencies of the crystalline lattice ions are typically lower, compared to the plasma frequencies, they fall in the infrared wavelength range.

Depending on the direction of vibration of the lattice cores, the polarization wave will assume longitudinal or transverse wave characteristics, respectively. However in bulk polar media the longitudinal polariton can be excited only at angles other than zero and with a polarization of the electric field in the incidence plane (i.e. in TM polarization).

We have recently developed a numerical/theoretical model to design metamaterials composed by a polar matrix and air inclusions. Combining homogenization techniques with the transfer matrix method for birefringent-layered materials, we modelled an effective medium layer where different inclusions' content, shape and orientation can be taken into account. The use of depolarization factors defined along the three main axes [2] allows to treat inclusions as oriented ellipsoids. The resulting dielectric constant display very different features in the directions of the three main axes making possible the tuning of spectral emissivity curves. One of the most intriguing feature of such nanostructured media is the random spatial alternation of inclusions and matrix, which offers the possibility to excite the longitudinal polaritons even at normal incidence and for the TE polarization (Fig. 1).

We have shown how anisotropic ellipsoids can be arranged, choosing both shape and orientation, so that the resulting spectral emissivity could match the emissivity peaks of hazardous chemicals for different polarizations of the emitted light. As an example, we designed a metamaterial-based device that matches the emissivity lines of two explosives, such as XRD (cyclotrimethylenetrinitramine) and TNT (trinitrotoluene), providing a double check in polarization that could increase accuracy of chemical sensors [3].

Many configurations can be considered by applying the same model in order to get also spatial modulation of infrared emissivity. We investigated a multilayer structure where the inclusions content is varying along matrix thickness to obtain strongly asymmetric emissivity fea-

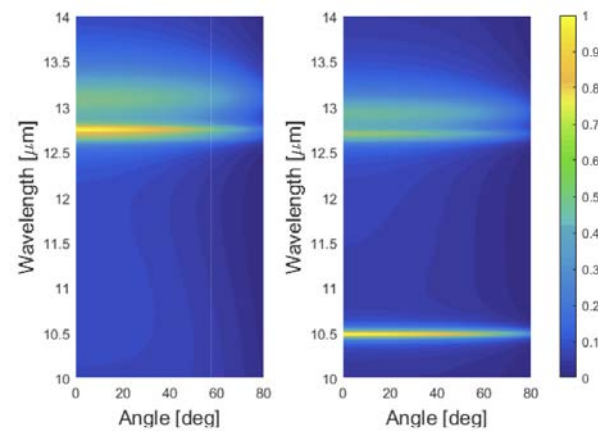


Figure 1: Emissivity spectra calculated for TE polarized fields as functions of wavelength and incidence angle for (a) a single SiC layer and (b) a SiC layer with 20% oriented air inclusions. SiC thickness is 1 micron, onto a Si substrate.

tures. Optimization of the porosity degree along the matrix thickness was performed in order to maximize the contrast between forward and backward infrared emission, in single SiC layer only few microns thick [4].

Furthermore, the typical ellipsoid of the refractive indices can be shaped as an uniaxial or even biaxial hyperboloid, in correspondence of negative values of the dielectric constant along one or two directions.

Taming and tuning the strength and the position of the phonon resonance in polar materials allows the design of versatile optical elements as basic elements for further developments of infrared filters, thermal diodes and thermal logic gates.

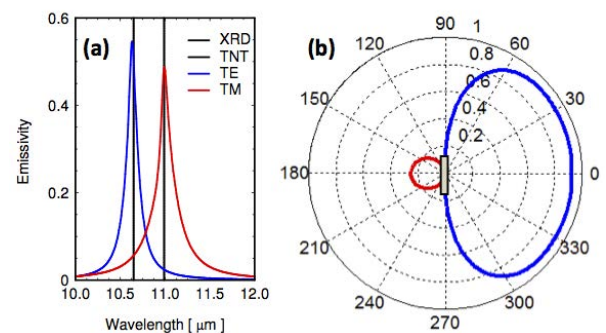


Figure 2: Spectral emissivity calculated for a system composed by oriented SiC inclusions into air matrix [3]. (b) polar plot of emissivity curve calculated at 10.48 micron, for a SiC layer 4 microns thick with graded air porosity [4].

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## P-21. Nondestructive testing by photoacoustic and photothermal techniques

*R. Li Voti, G.L. Leahu, G. Cesarini, C. Sibilìa*

Non-destructive testing (NDT) of materials plays a key role in industry where products have to be tested to verify the integrity and compliance with the standards. Since 1990 Photoacoustic and Photothermal laboratory (PA&PT lab) has been working to develop innovative instruments for NDT and quality control of materials. Recently in the period 2015-2017 the research at the PA&PT Lab has been applied to the NDT for military technologies [1,2], in both automotive [3] and aerospace industry, for photovoltaics applications, for nanophotonics [5,5] and nanophononic applications [6], and in agri-food industry.

As example of industrial applications developed with industrial partners is the device for the determination of the hardening depth profile in steels. The methodology involves the excitation of thermal waves and the detection of the reflected/backscattered thermal waves from obstacles and/or inhomogeneities, in analogy to conventional ultrasonic technologies. Several IR devices have been realised (PTR and TWADAR) for leading companies in the field of aerospace (AVIOGROUP) and automotive (BIFRANGI), to measure the cementation in hardened steels, in gears, ball bearings etc, alternatively to Vicker or Brinell tests. The devices are portable and fully integrated on a robotic arm for the local NDT of materials (in collaboration with MDM Metrosoft). Other recent strategic partnerships are with the Chinese organization in Nanjing for the inspection and quality control of products (NQI).

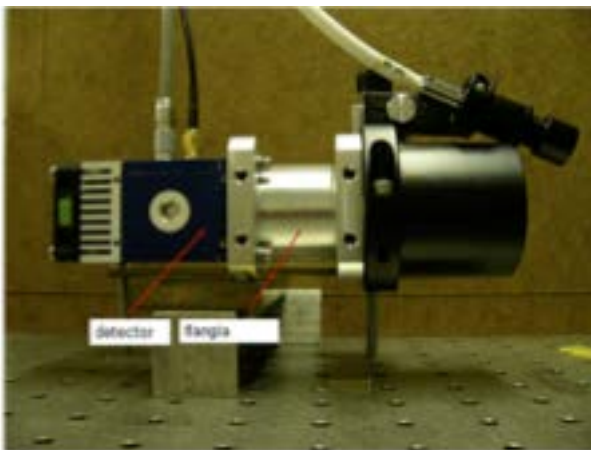


Figure 1: PTR compact device for measurements of gears.

The hardware of PTR device this system has been improved, made more compact, and integrated with mechanized and robotic arms for industrial needs [5] (see fig. 1). In particular the system uses a powerful IR laser working at 9W, modulated at a frequency ranging from

1Hz to 4kHz so to generate the thermal waves with a penetration depth from microns to millimetres. The waves penetrate the surface layer and are reflected from the inner martensite/austenite interface. The effects of thermal wave reflection are revealed by a Peltier cooled infrared sensor working in the range MIR 3-5  $\mu\text{m}$ . The software of the system has been developed so to retrieve the diffusivity/hardness depth profile by applying the Singular Value Decomposition tool to solve the severely ill posed inverse problem of the photothermal depth profiling.

In Figure 2 for example the hardness depth profile determined non-destructively by using the PTR (blue line) is compared with the one measured destructively, ex post, by Vicker test (red line). The excellent agreement between PTR and Vicker measurements has been confirmed on the whole set of samples, This is only an example of NDT techniques for industrial applications developed at PA&PT Lab.

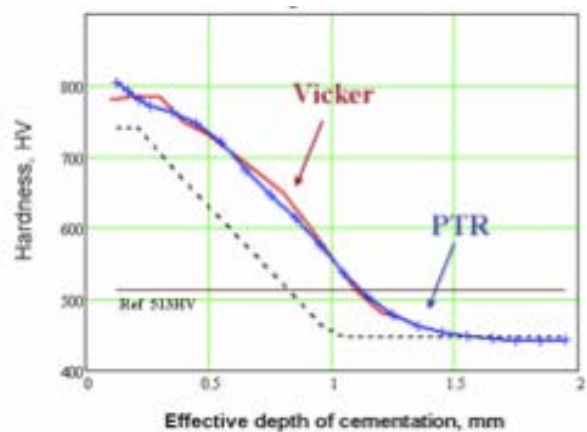


Figure 2: Hardened depth profiles in AISI9310 steels. Comparison between standard Vicker test (red line) and PTR NDT (blue line)

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## P-22. Molecular photonics: from linear and nonlinear optics in organic materials to biophotonics and liquid biopsy

F. Michelotti, A. Sinibaldi, A. Occhicone, E. Sepe

During the last three years, most of the research activities of the Molecular Photonics Group (MPG) have been focused on the development of a novel sensing technique [1] exploiting the characteristics of surface electromagnetic waves propagating at the interface between a truncated one-dimensional photonic crystal (1DPC) and an aqueous medium (Bloch surface waves, BSW). The studies have been carried out mainly in the frame of the EU funded project BILOBA (biloba.sbai.uniroma1.it) (N. 318035), which was coordinated by the MPG and involved 9 European academic and industrial partners. Other smaller national projects accompanied BILOBA during the period.

As shown in Fig.1a, the technique can operate in two complementary modes. It can sense in a label-free manner a refractive index change at the 1DPC surface by reflectometry under total internal reflection conditions (Kretschmann-Raether). Alternatively, it can resonantly excite fluorescent labels bound at the 1DPC surface and collect the BSW coupled and angularly dispersed fluorescence emission. The novel technique was applied to:

- Liquid biopsy for early cancer detection.** In this case (Fig.1b) the technique is used to detect the presence of specific protein biomarkers in a human plasma sample flowing at the 1DPC surface, in real-time and at very low concentration (pM). We immobilize at the 1DPC surface selected capture antibodies, which can specifically recognize and bind the target biomarkers, giving rise to a label-free signal. The use of a second labeled detection antibody, permits to introduce a fluorescence signal and to push resolution down to the limit of detection required for early cancer detection [2]. *In collaboration with Regina Elena National Cancer Institute (IRE/IFO) and Fraunhofer IOF (DE).*
- Fluid dynamics at boundaries.** Here (Fig.1c), the technique is used to probe in real-time and with nanometric resolution the fluid flow at a boundary wall of microfluidic channels, which are crucial in biosensing applications, under dynamic conditions [3]. *In collaboration with Fraunhofer IOF and IWS Institutes (DE).*
- Functional coatings for medical implants.** Here (Fig.1d), the technique was used to quantify the mass deposited in binary biomolecular coatings, constituted by fibronectin (FN), to stimulate endothelialization, and phosphorylcholine (PRC), for its hemocompatibility, which are two properties of relevance for cardiovascular applications [4]. *In collaboration with Laval University (CA).*

- Cavitation bubbles.** Here (Fig.1e), the technique is used to measure the pressure associated to a shock wave in very close proximity (100 nm) of a boundary surface and with high resolution (0.1 MPa). In the experiments, the shock wave was emitted by a cavitation bubble generated by a pulsed pump laser in water at different distances from the surface and for different pulse energies (manuscripts submitted). *In collaboration with Italian Institute of Technology-Center for Life Nano Science and Fraunhofer IOF (DE).*

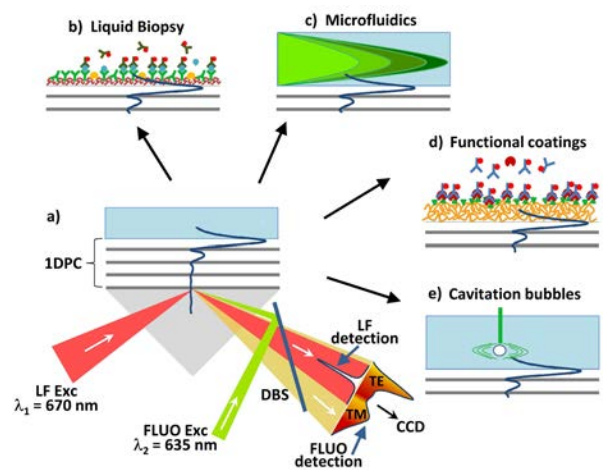


Figure 1: (a) Simplified sketch of the BSW based label-free and fluorescence sensing configuration. Applications: (b) specific probe antibodies bound at the surface capture biomarkers in human plasma, originating a label-free signal. Detection with a second labeled specific antibody permits to sense in the fluorescence mode; (c) BSW sense in label-free manner the liquid flow in proximity of a surface (100 nm); (d) the efficiency of functional coatings for human implants is tested by means of BSW; (e) pressure changes generated by a cavitation bubble in proximity of a surface is measured in a label-free manner.

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<https://web.uniroma1.it/labmp/>

## P-23. Cognitive- and bio-photonics

*E. Fazio, M. Alonzo, A. Belardini*

**Biophotons and signaling** The expression biophoton usually indicates the radiant emission of ultraweak light by living systems, non-thermal in origin, in the optical spectrum. In plants (as well as animals and humans) specific emissions were correlated to stresses, injuries or diseases; a number of investigations speculate on the role of electromagnetic radiation in signaling of cells and living entities. We have analyzed the emission of biophotons by Cannellini-Lingot beans (*Phaseolus vulgaris*). Seed coats [1] emit light as a consequence of the external environmental conditions, specifically in response to temperature, relative humidity and oxygen levels. Emission in different spectral band have been recorded according to the physico-chemical conditions. These observations led to the proposal that the seed coat acts as an environmental sensor available to seeds in the virtual dark beneath the soil to detect fluctuating environmental variables.

The emitted biophotons are conveyed to the embryo for controlling dormancy or germination by the seed coat, which acts as an optical collector for the emitted light [2]. The whole shape of the seed is constituted by several parabolic mirrors that collect the emitted light and re-focus it over the plumula of the embryo. Such biomorphism demonstrated that seed shapes are functionalized to favor the internal communication (signalling) of information from the surrounding environment to the embryo for the germination control.

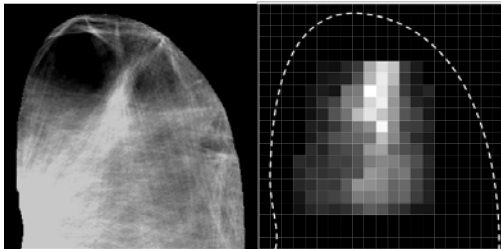


Figure 1: Theory and the experiment of biophotons emission and focusing by the seed-coat over the plumula of the embryo

**Stigmergic gates** Ethology has shown that animal groups or colonies can perform complex calculation distributing simple decision-making processes to the group members. For example ant colonies can optimize the trajectories towards the food by performing both a reinforcement (or a cancellation) of the pheromone traces and a switch from one path to another with stronger pheromone. This process is based on stigmergy, or the modification of the environment to implement distributed decision-making processes.

The procedure adopted by ants to search for food has been implemented in a photonic hardware [3-5] to reproduce such stigmergic signal processing. An innova-

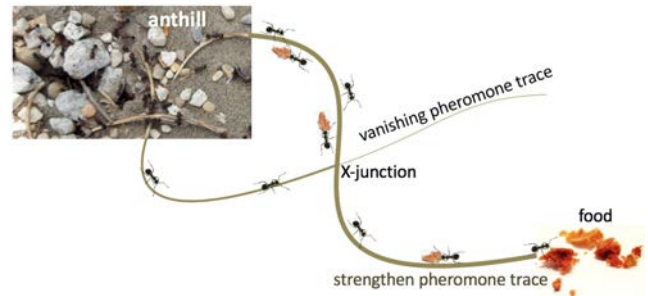


Figure 2: Ants looking for food leave trails of pheromone, which can be reinforced if food is found, or vanish if the research gives negative results.

tive, completely integrated X-junctions has been realized using solitonic waveguides, which can provide the two elementary ant's decision-making processes: follow a marked trail and switch from a less intense to a more intense path. Two laser beams generate two crossing channels within a nonlinear substrate in which the index of refraction is increased with respect to the bulk. These channels act as integrated waveguides within which optical information can be propagated (as happens for the ants that follow traces of pheromone already written). The proposed device is a X-junction with two crossing waveguides, that can be fully addressed by optical feedback. It can switch from symmetric (50/50) to asymmetric behaviors (80/20), vanishing unused output channels or reinforcing the used ones.

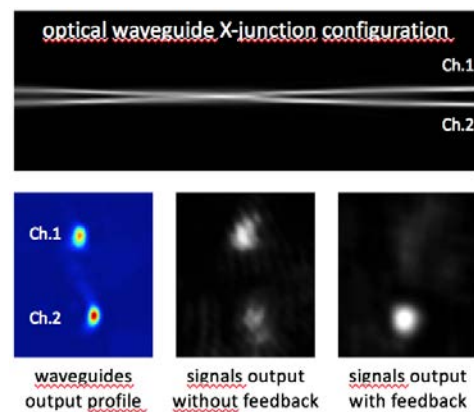


Figure 3: Simulation and experiment of an X-junction that can change performances according to an optical feedback injected in the network.

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## P-24. Non-destructive analyses and archaeometry

A.C. Felici, M. Piacentini, L. Pronti

The research activity has concerned archaeometric studies of several typologies of Cultural Heritages and the development of instrumentation for in situ non-destructive analyses. 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.

The activity can be summarized in the following research lines:

### • Pictorial materials and paintings

By using several non-destructive techniques different pigments, binding media and varnishes have been characterized with a particular attention to those pigments, such as for example lead, zinc and titanium whites, that are used as markers for dating artworks [1]. The results obtained on the pictorial materials have been tested on several paintings kept at the Accademia di San Luca (Roma) in order to verify their authenticity or to identify the substantial repaintings operated by their collector barone Lazzaroni.

### • Digital restoration of manuscripts

In collaboration with the Department of History, Cultures and Religions of Sapienza a research on the application of multispectral imaging to the digital restoration of degraded and faded manuscripts has been performed. Using ultraviolet radiation and collecting the images in different spectral ranges it was possible to enhance the readability of the text (Fig. 1) while illuminating the manuscript with visible light and collecting the images at longer wavelengths the hiding effect of brown spots covering the text was attenuated.



Figure 1: Digital restoring of a faded manuscript. Photography (left) and UV fluorescence image acquired using an interferential filter centered at 680 nm (right)

### • Archaeometric studies on archaeological materials

The archaeometric study of Roman coins from Pompei, started in the previous triennium, has been pursued. More than 500 coins from the mints of Ebusus, Massalia and Northeastern Iberia, together with the ones found in Pompei, have been analyzed by energy dispersive X-ray fluorescence spectroscopy in order to obtain information on the alloy and on the minor elements present in it. The huge amount of samples analyzed allowed to constitute a reference database and basing on it to suggest the provenance of the coins excavated in Pompei either from local mints as well as from foreign ones. In addition, fifteen coins from Pompei were analyzed with several non-destructive and micro-destructive techniques with the aim of characterize their conservation state [2].

### • In situ analyses as a support to archaeological excavations

Due to the portability of the instrumentation it was possible to participate to two excavation campaigns, one in Banbhore (Pakistan) [3] and the other in Estakhr (Iran) [4]. In this way it was possible to analyze in situ the findings just after they were excavated giving, in many cases, an immediate information to the archaeologists on the materials that constitute the objects and on their conservation state. Moreover, since the two excavation sites are abroad and the findings couldnt be transported in Italy, the presence on site of a diagnostic laboratory allowed a systematic archaeometric study, otherwise not possible, on a huge amount of ceramics and coins.

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## P-25. Radiation protection

*R. Remetti, G. Gandolfo, L. Lepore*

The research activity has two main objects: development and set-up of instrumental devices concerning radon issues, and development and set-up of devices for Special Nuclear Materials safety and security.

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) [1], [2]. One of the most important project was the design, realization and commissioning of a radon calibration chamber to test radon detectors (see Fig. 1). The main innova-

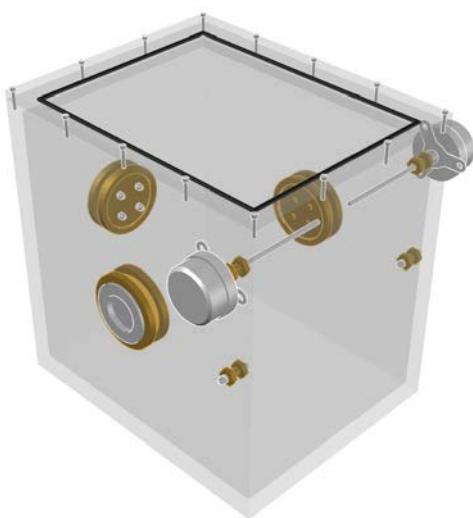


Figure 1: The radon chamber

tion is the way radon activity concentration is regulated inside controlled atmosphere. Unlike reference chambers with constant concentration, 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. Two ad-hoc transmitters monitor thermodynamic parameters inside the chamber: temperature, differential pressure and relative humidity. A microprocessor Arduino UNO WIFI, placed inside the chamber, provides the actuation for all the electrical devices in both circuits. The availability of the radon chamber opened the way to study and design an innovative radon detector belonging to the category of continuous radon progeny measuring instruments. It is called Radonino. The indoor air sampling is realized by micro diaphragm gas pump that forces the air flow through a millipore filter. The detector functioning has been based on the observation of radon progeny radioactive decay on the filter placed in front of a photodiode sensor. The

instrument is equipped with a custom amplification circuit and with a Multichannel Analyzer entirely relying on open source analogue to digital converter. The spectrometry algorithm has been specifically written in order to exploit the inner characteristics of a signals produced by detections of alpha particles. 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%. Further development will comprehend an increase of the prototype effectiveness, the usage of a professional high voltage supply and the introduction of metallic wire mesh filter to control the unattached fraction too [3].

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, envisaging its utilization in field applications. NAI is based on the detection of neutrons from induced fission on small amount, of the order of a few grams, of fissile material. The device exploits a portable neutron generator based on d-t fusion reaction, a polyethylene structure for reducing the neutron energy in order to maximize the fission cross-section, and an array of  $^3\text{He}$  proportional counters. 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. The activity required the preliminary MCNPX simulation of the d-t neutron generator [4], [5].

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# PhD programmes

## **Ph.D. in Mathematical Models for Engineering, Electromagnetics and Nanosciences**

The Ph.D. Course in Mathematical Models for Engineering, Electromagnetics and Nanosciences is aimed at preparing young graduated students to perform theoretical and applied research in the fields of Mathematics, Electromagnetics and Material Sciences. The program aims also at the development of scientific interaction between mathematics and applications.

Indeed mathematical modeling is actively employed in methods and problems studied in all curricula; for instance, we recall mathematical modeling of electrical conduction in biological materials with micro-structure, and the study of propagation of electromagnetic non-uniform waves in lossy media. On the other hand electromagnetics and materials science share the interest in innovative materials and systems (artificial materials, metamaterials, composites, nanostructured materials and components, photonic crystals, plasmonics, biological systems). The investigation of new materials can be carried out through the interaction of the electromagnetic radiation (in a wide spectral range, from the far infrared to the x-rays) and matter, by means of advanced optical and electronic spectroscopies, also making use of synchrotron radiation. In fact, electromagnetics and materials science share many techniques for analysis, simulation and characterization of the properties of such materials and systems, while the interest in their construction is specific to materials science.

## **Ph.D. in Accelerator Physics**

This Ph.D. programme, unique in Italy and therefore of national coverage, is oriented to the Accelerator Theory and Practice. It aims to prepare young researchers, profiting of the high level facilities both in the University and in the INFN, the National Institute for High Energy Physics.

The lectures are devoted to improve the knowledge in Physics, acquired during the graduation courses, to the principles of the Accelerator Theory and to their applications in the different domains of this science.

The students are offered both theoretical and practical lectures in the INFN laboratories. All the theoretical course can be attended, via e-learning, also from remote, to guarantee the national domain of the course.

The intrinsically international nature of the community behind Accelerator Physics implies that most of the students spend a significant amount of time abroad, in very high profile research infrastructures, like for instance, CERN.

# Laboratories and facilities

## List of laboratories and facilities

- L-1. Laboratory for structural, morphological, and electrochemical materials characterization
- L-2. LEOS - Laboratory of Electrochemistry and Organic Synthesis
- L-3. Laboratory of Molecular Electrochemistry and Mass Spectrometry, MEMaS
- L-4. Laboratory for thermal characterization of materials
- L-5. Physical Acoustics Lab
- L-6. Ultrafast Photonics Laboratory (U-Pho Lab)
- L-7. Laboratory for non-destructive analyses and archaeometry LANDA *Sebastiano Sciuti*
- L-8. Laboratory of PhotoAcoustic and Photothermal Techniques for nondestructive testing of materials – PA&PT LAB
- L-9. Molecular Photonics Laboratory
- L-10. Particle Accelerator Laboratory
- L-11. Laboratory of Radiation Protection
- L-12. Electron Microscopies and Nanoscopies (EMINA)
- L-13. SBAM (Scienze di Base Applicate alla Medicina) laboratory
- L-14. Nonlinear Photonics Lab
- L-15. Laboratory of physics of semiconductors and nano-structures
- L-16. Scientific computing facilities
- L-17. Departmental Library
- L-18. Mechanical Workshop

## L-1. Laboratory for structural, morphological, and electrochemical materials characterization

The laboratory houses the following equipment: 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, 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 shown in figure 2 g) and f).

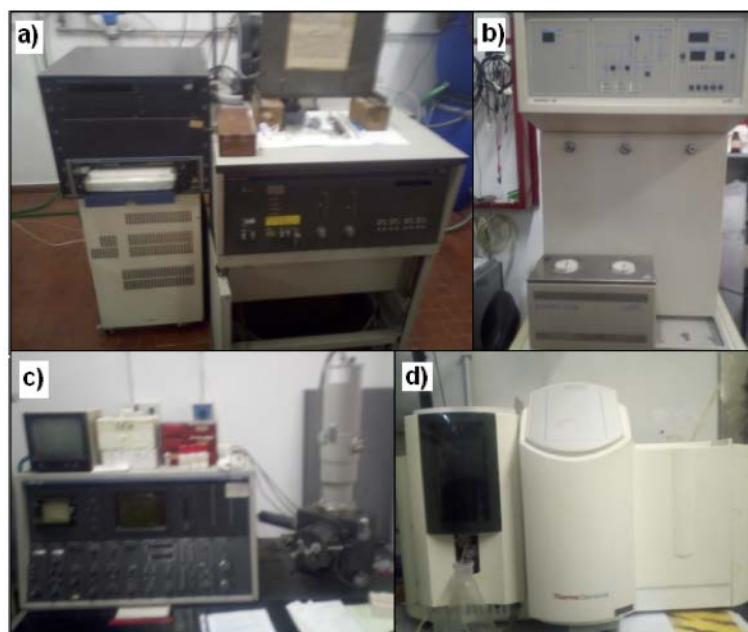


Figure 1: a) X-ray diffractometer, b) BET, c) Scanning Electron Microscope d) Atomic Absorption.

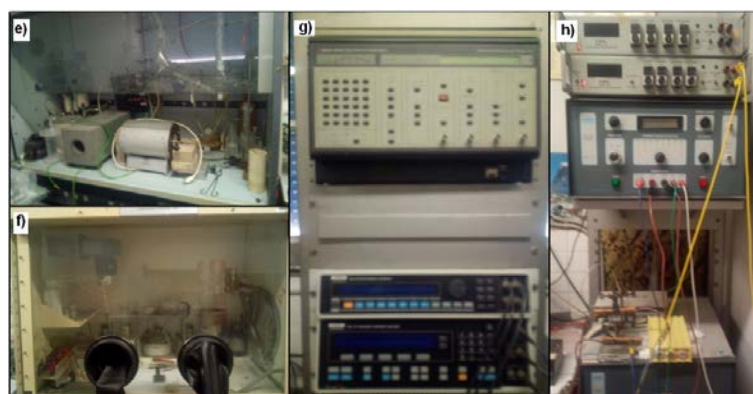


Figure 2: a) Chemical hood, b) Dry-box, c) Frequency Response Analyzer d) Galvanostat-potentiostats.

## L-2. LEOS - Laboratory of Electrochemistry and Organic Synthesis

### Facilities

LEOS is equipped with the following technical instrumentation:

- BRUKER Avance AC200 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 an Amel 566 function generator and an Amel 563 multipurpose unit
- Electrodes and microelectrodes for Voltammetric Techniques and Electrolysis (RVC, GC, Au, Pt, Zn, Fe, Mg, ITO,...)
- GC-MS Hewlett-Packard 5890 series II Gas Chromatograph coupled with a Hewlett-Packard 5871 series II quadrupole Mass selective detector
- UltraSound high-energy sonicator
- Ultrasound bath apparatus
- complete experimental setup for chromatographic techniques (TLC, Flash)
- complete experimental setup for synthetic organic chemistry
- Bchi melting point apparatus
- Schlenk apparatus for manipulation and synthesis of air-sensitive compounds (vacuum or inert gas atmosphere)

### LEOS Expertise

The group has more than twentyfive 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. In the laboratory various instruments are available for basic and applied electrochemical studies, for preparation and for some spectroscopic characterizations of the materials. The group has always carried out training of young researchers in the field of organic and electroorganic synthesis.



Figure 1: Left panel: NMR spectrometer; right panel: electrochemical apparatus

### L-3. Laboratory of Molecular Electrochemistry and Mass Spectrometry, MEMaS

The laboratory located at RM017 P01 L022 houses instruments used to study the electrochemical behaviour of substrates of interest: potentiodynamic methods (Voltammetry) are performed by a three-electrode multipolarograph AMEL 472 coupled with a digital x/y recorder AMEL 863; controlled potential electrolyses (CPE) are performed by a potentiostat AMEL 552 coupled with an integrator AMEL 731 and an x/y recorder LINSEIS L250E. CPE are mainly carried out using a three-electrode UV-vis cell modified for spectroelectrochemistry and an Agilent 8453 diode array spectrophotometer (see Fig. 1).

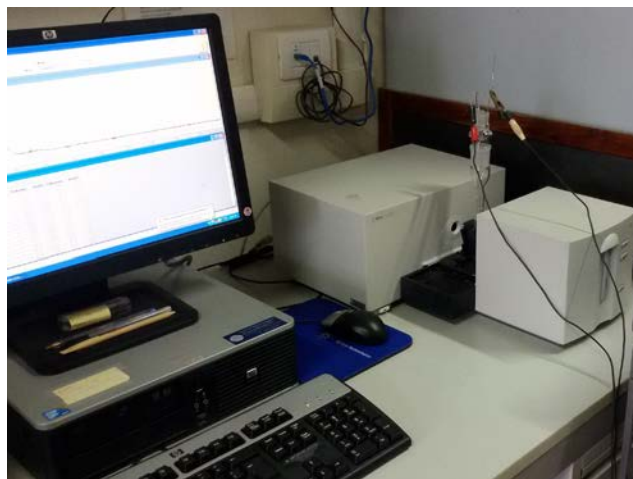


Figure 1: UV-vis ChemStation for spectroelectrochemistry.

The Laboratory located at RM017 PS1 L022 houses instruments for analytical purpose, as detection, determination and characterization of compounds in/from different matrices. The apparatus is composed of a High Performance Liquid Chromatography HPLC separation module 1525 $\mu$  Waters, linked to a photodiode array detector Waters 996 PDA and to a Quattro Micro Tandem MS-MS with an electro-spray interface ESI Waters (Micromass, Manchester UK) as mass spectrometry detector (see Fig. 2)



Figure 2: HPLC-PDA-MS/MS Waters system.

## L-4. Laboratory for thermal characterization of materials

For more than 20 years we have been dealing with thermal analysis with particular reference to the assessment of thermal stability and lifetime prediction of a wide range of materials. The laboratory, located in room 1.15 of the raised floor of building RM017, is equipped with the following apparatuses:

STA 625 Stanton Redcroft simultaneous thermoanalyzer, for thermogravimetric and differential scanning calorimetry measurements for condensed phase materials, in a controlled gas atmosphere (argon, air, carbon dioxide) up to 625C;

STA 1500 Stanton Redcroft simultaneous instrument (on loan for use by the Department of Chemistry of Sapienza University of Rome), for thermogravimetric and differential thermal analysis measurements for materials in the condensed phase, in a controlled atmosphere (argon, air, carbon dioxide) up to 1500C;

Nicolet Impact 410 Fourier Transform Infrared (FTIR) spectrophotometer equipped with standard accessory and diffused reflectance.

## L-5. Physical Acoustics Lab

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

Research activities are primarily focussed on the following two subjects:

### 1. Acoustic waveguides

The question: “*How much time it takes for a quantum particle to tunnel through a barrier?*”, is a basic problem in quantum mechanics, being today also of technological importance. Backward propagating Lamb waves (plate modes) are used to experimentally investigate the transit time of phonons through a potential barrier. In backward wave propagation, the direction of the energy flux, or group velocity, is antiparallel to the phase velocity direction, or direction of motion of the phase fronts. Backward wave propagation has seen a growing interest in both acoustic and optics due to fact that it offers new ways to manipulate acoustic and optical fields and leads to non-intuitive physical effects such as anomalous (negative) reflection and refraction phenomena on which, for example, acoustic cloaking effect relies.

### 2. Biomedical ultrasonics

Ultrasound attenuation caused by dispersed solutions of microbubbles and nanobubbles, is an important physical parameter that is measured in the Lab to improve the backscatter properties of such systems that are increasingly used as ultrasound contrast agents (UCAs) in clinical applications. 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.

High frequency shear acoustic waves biosensors in a Quartz Crystal Microbalance (QCM) measuring system are used for non-invasive, label-free and highly sensitive chemical and cell biology studies with a special focus on cell-substrate interactions. Measurements on the rheological properties of biological fluids are also carried out.

Lab equipment includes:

- High-frequency broadband ultrasonic pulse-echo measuring system with fourier transform spectroscopy analysis for nondestructive evaluation of biological samples;
- Two computer-controlled 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  $\mu\text{m}$ ). Vibrational amplitude map are generated with a field-of-view up to 5  $\text{cm}^2$ ;
- Network analyzer for real-time impedance measurement of ultrasound piezoelectric transducers;
- Computer-controlled Quartz Crystal Microbalance (QCM);
- Temperature-controlled apparatus for the study of cavitation and single-bubble sonoluminescence.

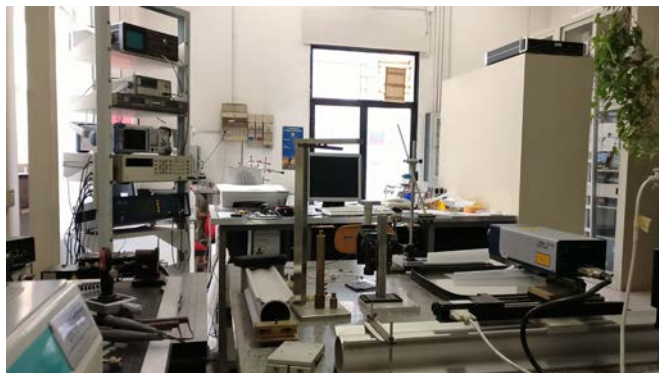


Figure 1: The Physical Acoustics Lab at SBAI Department

## L-6. Ultrafast Photonics Laboratory (U-Pho Lab)

The Ultrafast Photonics Laboratory (U-Pho Lab) gathers equipment, expertise and experiments in the framework of linear and nonlinear optics, environmental monitoring, high-resolution single-photon luminescence and optical sensing. It was established in 1992 and since then it has performed both fundamental and applied researches in collaboration with private companies and other research laboratories. Its main activity regards the realization of innovative self-assembled integrated photonic circuits. Such research is going towards the design of innovative cognitive configurations of photonic devices. Noteworthy researches regard also the nonlinear characterization of nanostructured media, single-photon counting of light emission by biological structures and optical very-early diagnostic of Alzheimer disease. Since 2008 the Laboratory has generated a spin-off company, called OptSensor s.r.l., which performed innovation in the framework of optical sensing for chemical industries and environmental pollution detection.

**Instrumentation.** The Ultrafast Photonics lab is a complete optical laboratory. Thus, any kind of transmission /reflection/absorption/emission test can be performed on materials. U-Pho Lab possesses many lasers and LED sources of different wavelengths, ranging from violet to infrared, from CW to femtosecond regime. Slow and fast detectors are present as well as many devices for beam-quality analysis, like optical spectrum analyzers of beam profilers. U-Pho Lab has a 20-year experience in imaging and characterizing laser beams. The laboratory is equipped also with very sensitive detectors and photon-counting systems with ultralow dark noise (?1015 counts/sec). A custom monitoring station for PM1-PM2.5-PM10 particulate pollution has been built in the lab and perfectly working. Using an innovative optical detection method, it allows to perform fully-automatic and fully-programmable monitoring loops of particulate pollution, both indoor and outdoor.

**Work for third parties.** U-Pho Lab provides a number of activities outwards, and more specifically:

- A) laser safety training courses;
- B) design of laser-safe laboratories and procedures;
- C) design of custom optical systems and sensors;
- D) characterization of optical materials;
- E) technical consulting on optoelectronic optical and photonic systems, as well as on innovative sensors based on light;
- F) forensic technical consulting in the optical and laser fields, and in the field of road accidents for the kinematic and dynamic reconstruction of major car crashes.

## L-7. 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.

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 an 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.

- **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 LEDs 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 radiography system**

A portable system that allows to perform a radiography of the artworks without moving them from the place where they are kept.

<https://web.uniroma1.it/landa>

## L-8. Laboratory of PhotoAcoustic and Photothermal Techniques for nondestructive testing of materials – PA&PT LAB

In the PA&PT Lab, located in Building RM008, floor PS1, Room L012, 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: measurements of thermal diffusivity of materials; optical and infrared reflectance, 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 nanophonics.

### Laboratory equipment

- 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. Photo-multiplier. Infrared Camera 8-14  $\mu\text{m}$ .
- Electronics: 2 Lock-in amplifiers. Digital oscilloscope Tektronix- - Microvoltmeter HP
- Mechanics: 2 optical tables (Newport). Automatized rotation and translational stages.
- HW and SW: 4 desk-top PCs. Software LabView.



Figure 1: From left to right: Infrared radiometric set-up; photothermal detection apparatus; photoacoustic cell.

## L-9. 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 pursue 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.

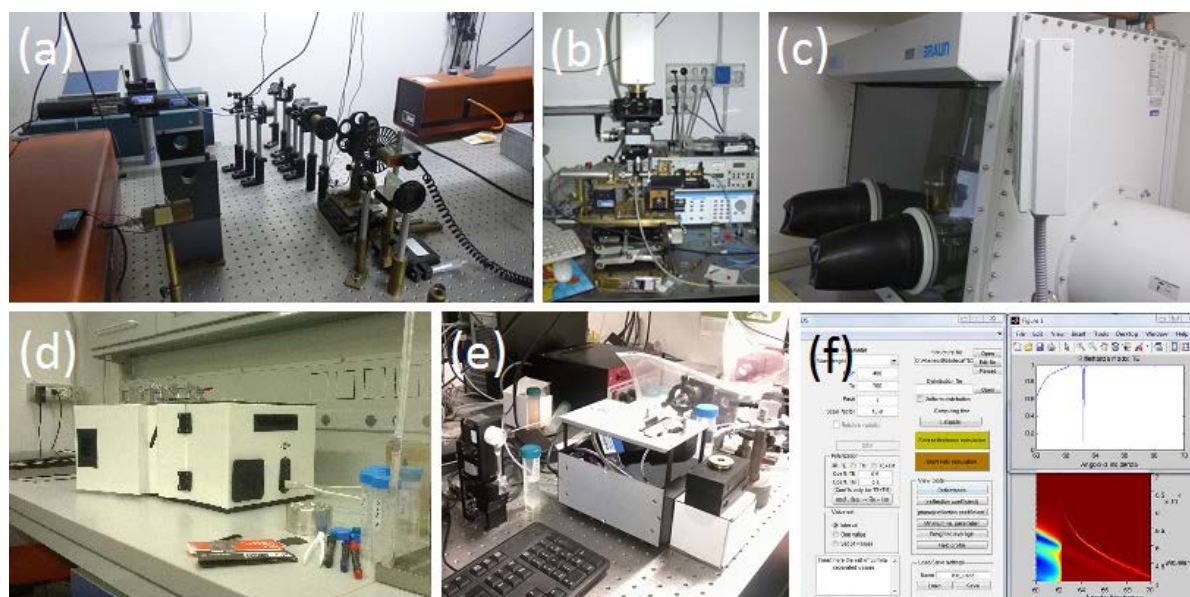


Figure 1: (a) Custom benchtop optical setups, (b) Integrated photonics setup, (c) Glove-box, with DC sputtering and spin coating systems, (d) BSW early cancer biomarker detection platform developed in the project BILOBA, (e) Infrared Surface Plasmon Resonance platform, (f) Custom and commercial tools 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);
- modelocked Nd:YAG laser (1064nm, SH 532nm,  $f=76\text{MHz}$ , 100ps), dye laser (R6G band,  $f=0.147\text{-}38\text{MHz}$ , 1ps), Q-Switched Nd:YAG laser (1064nm, SH 532nm,  $f=1\text{-}10\text{Hz}$ , 6ns);
- 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);
- CW sputtering (gold) and spin coating systems;
- Range of didactic kits used in the optics and photonics courses, including a WEB accessible ellipsometer (<https://remotelab.ing2.uniroma1.it/>)

<https://web.uniroma1.it/labmp/>

## L-10. Particle Accelerator Laboratory

The laboratory is devoted to the design and measurement of Radio Frequency (RF) devices for modern particle accelerators. Those devices are designed with the aid of standard software, widely used in modern RF engineering, e.g. Ansoft-HFSS or CST-Microwave Studio; the dynamics of particles inside those devices is also optimised with dedicated tools widely used in the Accelerator Physics community (e.g. TSTEP). The laboratory is equipped with servers dedicated to those softwares.

Vector Networks Analysers (VNA) are used to bench measure any particle accelerator RF device, e.g. accelerating and deflecting structures, beam position monitors, resonant cavities as well as low power electronics. The laboratory hosts four VNAs operating from few kHz to 20GHz, as well as the necessary mechanical and electronic calibration kits. High frequency signal generators, spectrum analysers and calibrated antennas are also available for Electro-Magnetic compatibility measurements. Typical RF devices, such as amplifiers, attenuators, power splitters, directional couplers, filters, high accuracy cables are also present covering the 20GHz range. All our instruments can be remotely controlled with standard application (such as Labview and Matlab) as well as integrated in complex bench measurements requiring the synchronisation of the instrument with external devices (e.g. step motors).

The laboratory can perform complex, general purpose RF measurements (e.g. Time Domain Reflectometry) as well as bench measurements typical of the accelerator engineering, e.g. coaxial wire or bead pull techniques. The Coaxial Wire method is used to estimate the coupling impedance of accelerator devices, a quantity affecting the beam stability in accelerators. Bead pull is used to measure the electro-magnetic field acting on the particles both in resonant and non resonant devices; the perturbing object can be calibrated in dedicated pillbox cavities.

Most of the devices designed and measured in the accelerator laboratory are standard S-band (3GHz) devices, in particular deflecting cavities; we also measured and tuned C band (6GHz) travelling wave devices before the high power tests. We also designed and measured different accelerating multi-cell cavities in X Band (12GHz). All our activity is in tight collaboration with INFN Laboratori Nazionali di Frascati, where such devices are used in operating accelerators.

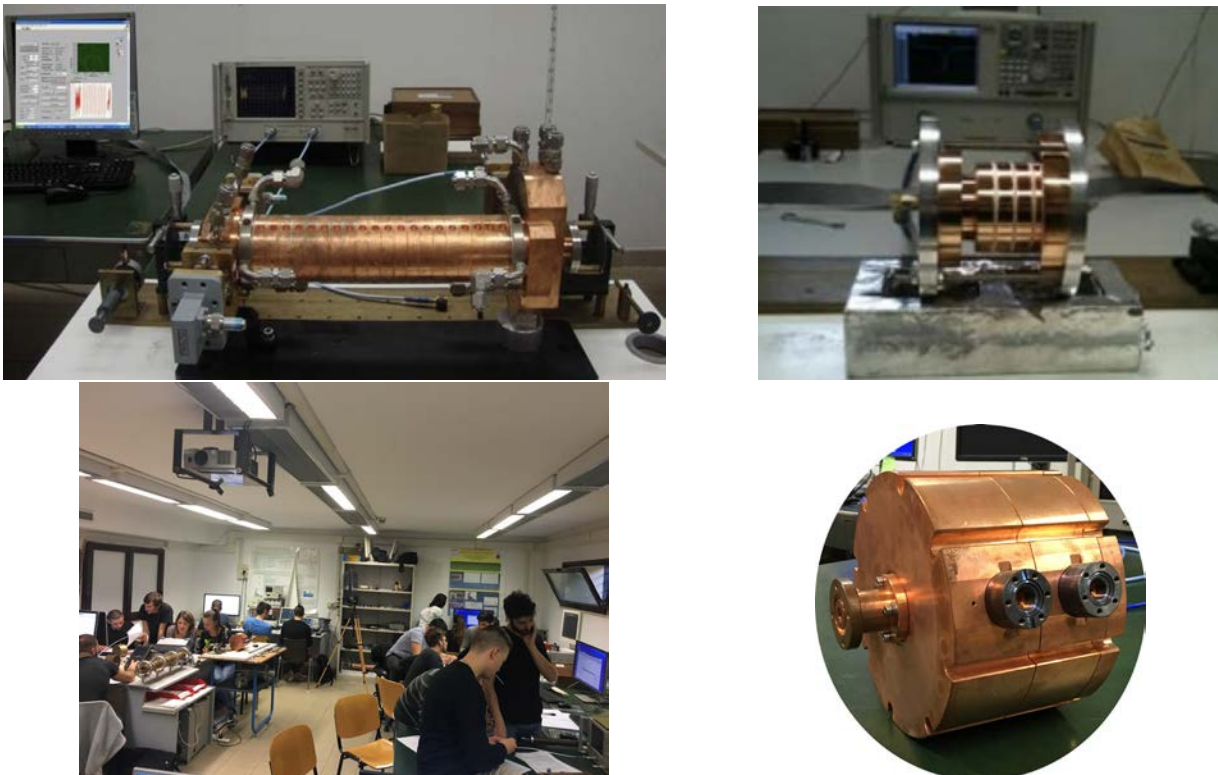


Figure 1: Bead pull measurement of C band travelling wave device (top left picture), X band standing wave multi-cell cavity (top right picture), students working in the laboratory for the microwave measurement laboratory course (bottom left picture) and S band multi-cell deflecting cavity (bottom right picture)

## L-11. 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). Laboratory hardware includes:

- AlphaGUARD, for measurements of radon concentration in air;
- AquaKIT, coupled with AlphaGUARD, for measurements of radon concentration in drinking waters;
- Tracerlab BWLM-PLUS-2S, for measurements of radon-related potential alpha energy concentration in air (PAEC), Figure 1;
- 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, for low-cost alpha spectrometry of samples;
- Radonino detector, for low-cost measurements of radon-related potential alpha energy concentration in air (PAEC);
- 3D printer for self-building of components;



Figure 1: The Tracerlab system for measuring attached and unattached radon decay products

The Laboratory endowment also includes the following software: Monte Carlo N-Particle eXtended code MC-NPX, for shielding calculation, detector simulations and radiation-based techniques optimization; GoldSim Simulation software for radionuclide dispersion and transport through environmental pathways; Canberra suite Genie2000 and Ortec Gamma Vision software for gamma spectrometry.

## L-12. Electron Microscopies and Nanoscopies (EMINA)

Facilities of EMINA scanning probe microscopy (SPM) laboratory include a set of three SPM platforms (NT-MDT, Russia), i.e., two atomic force microscopy (AFM) and one scanning tunneling microscopy (STM) setups. In particular, AFM platforms can perform standard morphological characterizations in tapping and contact mode both in air and in liquid, including also the facility for mechanical, electric and magnetic characterizations.

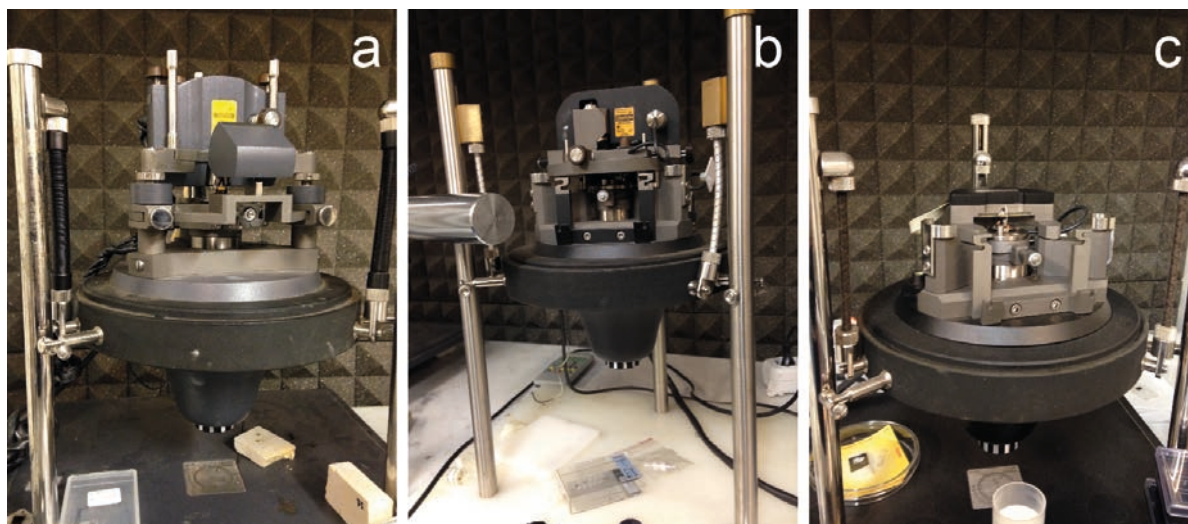


Figure 1: SPM setups available at EMINA: (a) AFM with the facility for mechanical characterizations, (b) AFM which can operate both in air and liquid, (c) STM setup.

## L-13. SBAM (Scienze di Base Applicate alla Medicina) laboratory

The SBAM (Scienze di Base Applicate alla Medicina) laboratory is a facility hosting the tools and necessary equipment for the development of state of the art particle and radiation detectors with applications in the Medical Physics field. Several detector, of different radiation types, are available in the laboratory or can be assembled in the SBAI mechanical workshop. Figure 1 shows the laboratory during the assembly and test of a multi-purpose detector setup aiming to the simultaneous detection of prompt photons, PET annihilation photons and charged fragments produced by the interactions of carbon ion beams used in particle therapy treatments with thick targets.



Figure 1: SBAM laboratory during the assembly of the table-top experiment performed at Heidelberg in 2014. The experiment setup foresaw the simultaneous detection of prompt photons, PET annihilation photons and charged fragments produced by the interactions of carbon ion beams used in particle therapy treatments with thick targets.

The SBAM lab is equipped with different types of detectors (see Figure 2 for example) that can be used to measure incoming radiation of the energy of interest for Medical Applications, especially in Particle Therapy. The full data detection chain can be exploited within the SBAM facility: the detector construction and test, the electronics development, the readout implementation and the data acquisition and analysis can be performed using the hardware and software tools available.

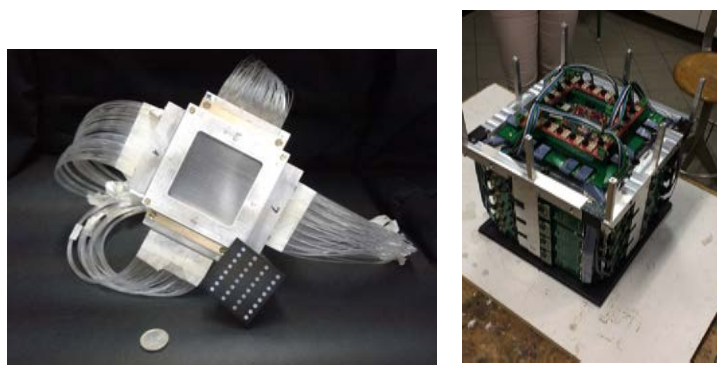


Figure 2: (Left) Plastic scintillator detector optimised for ToF measurements. The readout is performed using fibres. (Right) Dose Profiler detector: a charged particles tracker optimised for the monitoring of Particle Therapy treatments performed using carbon ions.

<http://arpg-serv.ing2.uniroma1.it/arpg-site>

## L-14. Nonlinear Photonics 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 information" 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.
- It is also equipped with different laser sources, monochromators, spectrum analyzers and tools for experimental investigations in both of linear and nonlinear optics.

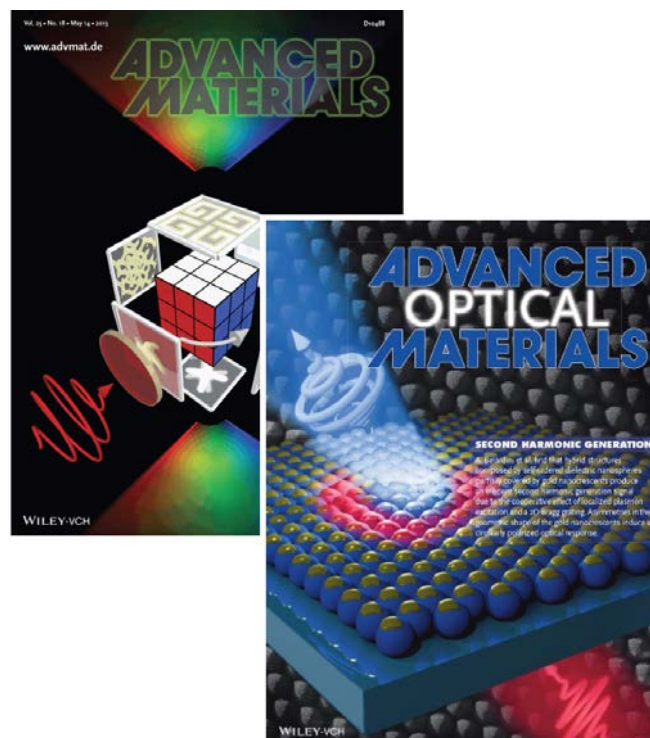


Figure 1: Simulations and Experiments on nonlinear artificial chiral materials

## L-15. Laboratory of 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 and four servers for high performing computing (HPC) (see Fig.1(a)). Structural characterization of materials and nano-structures is mainly performed by Transmission Electron Microscopy (TEM), optical microscopy and Reflection High Energy Electron Diffraction (RHEED). The laboratory owns two electronic microscopes, the first one operating in transmission at 160 kV [Fig. 1(b)], the other equipped with a high resolution reflection stage for RHEED measurements and shown in Fig. 1(c). The laboratory owns also the entire equipment needed to build and prepare samples for TEM, including the final ion milling stage [Fig. 1(d)].

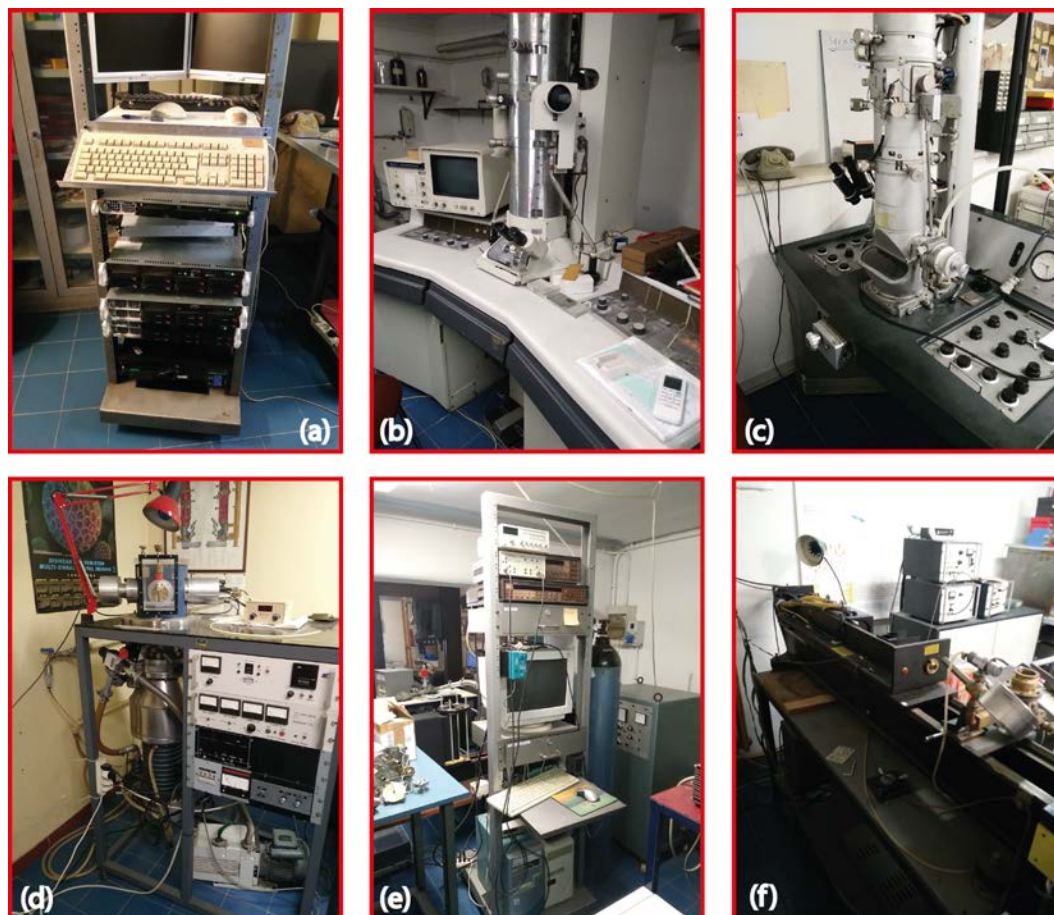


Figure 1: Some of the main apparata owned by the laboratory

Concerning the electrical and the electronic characterization of materials, the laboratory is equipped with a set-up for measuring a variety of 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. 1(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. 1(f)].

## L-16. Scientific Computing Facilities

SBAI researchers perform scientific computations both using external High Performance Computing resources (e.g. at CINECA and ENEA-CRESCO) and in-house facilities.

A first in-house facilities is a Scientific Computing Laboratory, located at the ground floor of the building RM002. The laboratory activity started in 2012. The laboratory was originally equipped with two Server Sun Fire – X2100 M2 rack 1U – 1 AMD Opteron modello 1210 – DDR2–667 4Gb. More recently one Server SuperMicro rack 2U – Double Processor Intel Xeon E5620 – DDR3 1333Mhz 24Gb has been added. This server is equipped with the Scientific Linux release 6.10 (Carbon) system. In the past few years the laboratory has been mainly used as a support for the mathematics research lines, mainly as an instrument to run Monte Carlo simulation and to perform numerical studies of partial differential equations. The laboratory has been used not only by the researchers of the Department, but also by many PhD students of the PhD school Mathematical Models for Engineering, Electromagnetics and Nanosciences.

A computational infrastructure with a total of more than 250 cores and four servers for high performing computing (HPC) is hosted by the Laboratory of physics of semiconductors and nano-structures.

The Department has also designed and assembled a simulation server with four GPUs running in parallel for raytracing applications and for developing new-generation Monte-Carlo codes. Thanks to a closed-circuit liquid cooling system, the GPU cards can sustain continuous operation, since the temperature of the computing hardware is kept well below 45 Celsius. For the described applications, the server has a performance comparable to that of a conventional cluster of more than 1000 CPU computing nodes.



Figure 1: Closed circuit liquid cooled GPU server.

## L-17. Departmental Library

The Library of Basic and Applied Sciences for Engineering (SBAI) is divided into three topical sections (Mathematics, Physics and Chemistry) holding about 20,000 volumes, 200 journals (between current and closed) and online-only periodicals (SIAM Journals, OSA Journals, Royal Chemical Society). In addition the Library houses a number of collections of considerable value (including Laurence donation and Martinelli donation).

The library has four reading rooms. The largest one with seventy seats was inaugurated in May 2017 as a 24 hours service. The room is accessible after normal opening hours using a personal magnetic card. Students can request access to the facility directly via the Infostud system.



The H24 studying and reading room.

The three smaller rooms are reserved for specialist consultation, and reach a total of forty-three study seats. The Library also provides access to people with disabilities and offers two terminals for consulting catalogs and digital bibliographic resources.

The Library makes it available to the specialized user a study room for the consultation of mathematical series, equipped with a workstation connected to the Internet.

The Library adheres to the National Library System (SBN), the National Archive of Periodicals (ACNP), the inter-library loan service SBN / ILL, the network Inter-library document exchange (NILDE) for the mutual exchange of articles and documents scientific among libraries.

The SBAI Library offers consultation services, bibliographic assistance, supply of scientific articles and interlibrary loan to all users. The Library assists in carrying out research activities mainly on the topics of chemical, physical and mathematical disciplines that present a significant application aspect.



Students in the reading room.

<http://www.sbai.uniroma1.it/strutture/biblioteche>

## L-18. Mechanical workshop

The Department's mechanical workshop (Fig. 1) is equipped with several traditional machine tools including a lathe, two vertical milling machines, column drills of different sizes, band saws, a shear. An FDM 3D printer is also available. It has been used to produce a variety of objects, from small optical media to complex research prototypes.

The workshop, albeit with traditional machines, actively supports research by producing functional prototypes of considerable complexity and automation, as well as mechanical accessories for the various work groups. It also provides assistance to departmental educational laboratories. In addition, the mechanical workshop assists researchers in the design and implementation phase of the CAD part of the projects.

Recently produced prototypes of considerable complexity include a detector and scintillating dose-profiler fibers (Fig. 2), a thermobalance for the determination of the vaporization and sublimation enthalpy (Fig. 2) a remote control system for various optical experiments with revolver system; a beam monitoring system for the ELI accelerator.



Figure 1: Partial view of the workshop

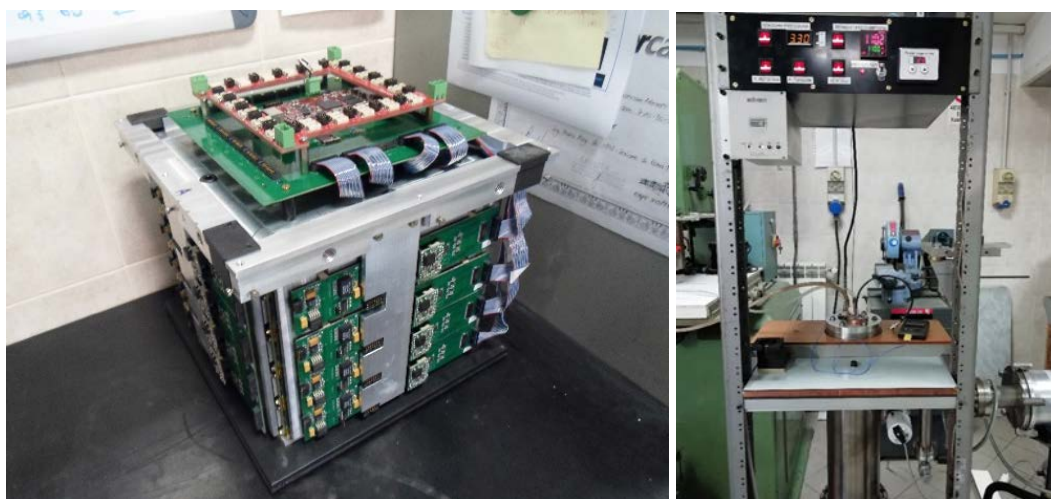


Figure 2: detector and scintillating dose-profiler (left); thermobalance (right)

# Grants



## International competitive grants

### FP7-ICT

BILOBA: Bloch electromagnetic surface wave Bio-sensors for early cancer diagnosis, Grant agreement ID: 318035, Oct. 1, 2012 – Dec. 31, 2015  
Principal investigator: F. Michelotti  
Local fund: 1 264 107 Euro

### H2020-EU.1.4.1.1 - INFRADEV

Eupraxia, European Plasma Research Accelerator with eXcellence in Applications, Grant Agreement ID: 653782, Nov. 1, 2015 – Oct. 31, 2019  
Local coordinator: A. Mostacci  
Local fund: 5 770 Euro

### H2020-WIDESPREAD-04-2017-TeamingPhase1

ENSEMBLE3: Centre of Excellence for nanophotonicS, advancEd Materials and novel crystal growth-Based technoLogiEs, Grant agreement ID: 763798, Sep. 1, 2017 – Aug. 31, 2018  
Local coordinator: C. Sibilia  
Local fund: 28 000 Euro

### H2020-EUROfusion Enabling Research Project

Preparation and Realization of European Shock Ignition Experiments, project AWP17-ENR-IFE-CEA-01, grant agreement No 633053, Jan. 1, 2017 – Dec. 31, 2018  
Local coordinator: S. Atzeni  
Local fund: 33 750 Euro

## International Academic agreements

### Erasmus Mundus

ARCHMAT: Erasmus Mundus Master in ARCHaeological MATerials  
Coordinator: G. E. Gigante  
Local fund: 135 970 Euro

### International agreement with Peru universities

Coordinator: G. E. Gigante  
Local fund: 5 000 Euro

### International agreement with Chile universities

Coordinator: A. Pistoia  
Local fund: 5 000 Euro

### International agreement with Pakistan

Coordinator: G. E. Gigante  
Local fund: 4000 Euro

## National competitive grants

### PRIN 2011-2011 (Feb. 1, 2013 – Feb. 1, 2016)

INSIDE: Soluzioni innovative per la dosimetria in-beam in adroterapia oncologica  
Principal investigator: V. Patera  
Local fund: 148 572 Euro

### PRIN 2012 (Mar. 8, 2014 – Mar. 8, 2017)

Laser-driven strong shock waves  
Principal investigator: S. Atzeni  
Local fund: 75 210 Euro

### FIRB 2012 (Mar. 21, 2013 – Mar. 21, 2016)

Generazione di fasci di elettroni di alta brillantezza con acceleratori a plasma

Principal investigator: A. Mostacci  
Local fund: 181 583 Euro

Rita Levi Montalcini grant (Apr. 1, 2014 – Mar. 31, 2017)  
Rapida accelerazione di un fascio di alta brillantezza di elettroni per mezzo dell'accelerazione a plasma indotta da laser nel gas contenuto in capillari  
Investigator: M. Petrarca  
Local fund: 78 643 Euro

FFABR MIUR Grants 2017  
19 grants, for a total of 57 000 Euros

## Funding by National Research Institutions

Collaboration with ENEA  
Progetto PAR  
Principal investigator: M. Pasquali  
45 800 Euro

INFN-SBAI Agreement  
SBAI Principal Investigator: L. Palumbo  
30 000 Euro

SBAI-CNR agreement for L. Schio grant  
13 641 Euro

GNAMPA and INDAM-GNFM grants  
several grants to the groups of Mathematics, for a total of about 10 000 Euros

## Sapienza competitive grants

We list here *Large size projects*, *Medium size projects* and *Interdisciplinary projects*. In addition to these grants SBAI researchers obtained a number of smaller grants, which can be summarized as follows:

2015:

*Small projects*: 4 grants, for a total of 21 000 Euro  
*Organization of conferences*: 1 grant, 4000 Euro  
*Research start grants for post-docs*: 6 grants, for a total of 7 500 Euro  
*Visiting professors*: 9 grants, for a total of 72 700 Euro

2016:

*Small projects*: 8 grants, for a total of 34 000 Euro  
*Organization of conferences*: 2 grant, 8000 Euro  
*Research start grants for post-docs*: 6 grants, for a total of 6 000 Euro  
*Visiting professors*: 6 grants, for a total of 27 000 Euro

2017:

*Small projects*: 5 grants, for a total of 17 000 Euro  
*Organization of conferences*: 1 grant, 1000 Euro  
*Research start grants for post-docs*: 8 grants, for a total of 10 500 Euro  
*Visiting professors*: 6 grants, for a total of 41 000 Euro

## 2015 Large size projects

Asymptotics of inhomogeneous diffusion problems

Principal investigator: D. Andreucci

32 000 Euro

Beam dynamics and collective effects in the CERN Future Circular Collider electron accelerator

Principal investigator: M. Migliorati

30 000 Euro

## 2015 Medium size projects

Liquidi ionici imidazolici dicationici: stabilità e reattività Principal investigator: I. Chiarotto

13 000 Euro

Plasma models: bridging the gap between kinetic and hydrodynamic simulations

Principal investigator: S. Atzeni

13 000 Euro

Realtà aumentata per la visione e il riconoscimento ottico in tempo reale di arterie, vene e nervi in chirurgia

Principal investigator: E. Fazio

11 000 Euro

Progettazione, caratterizzazione e realizzazione di metasuperfici plasmoniche su VO<sub>2</sub> per il controllo ed emissione di radiazione infrarossa.

Principal investigator: R. Li Voti

9 000 Euro

Aspetti geometrici di equazioni ellittiche semilineari

Principal investigator: A. Pistoia

11 000 Euro

Misura del profilo di dose in protonterapia: studio della microstruttura temporale del fascio terapeutico del centro di Trento e della sua influenza sulla misura del flusso di particelle secondarie

Principal investigator: A. Sciubba

36 450 Euro

Frattali dinamici e applicazioni

Principal investigator: M. A. Vivaldi

9 000 Euro

## 2015 Interdisciplinary projects

Mitigating the potential impacts of climate change and natural hazards on Cultural Heritage Sites, Structure, Materials and Artefacts (CHSSMA)

Principal investigator: G. E. Gigante

30 000 Euro

## 2016 Medium size projects

Ion and electron kinetic effects in laser-driven inertial fusion plasmas

Principal investigator: S. Atzeni

14 000 Euro

Determinazione in tempo reale della viscoelasticità ematica mediante metodi ultrasonor

Principal investigator: A. Bettucci

10 000 Euro

Asymptotical methods in linear and nonlinear evolution problems

Principal investigator: S. Carillo

13 000 Euro

Scambio termico radiativo alla nanoscala: controllo dinamico della densità di flusso termico tra sistemi ibridi composti da nanoantenne plasmoniche e *phase-change materials*

Principal investigator: M. Centini

10 000 Euro

Modelli singolari e degeneri di diffusione non lineare

Principal investigator: V. De Cicco

33 600 Euro

Reazione di Willgerodt-Kindler indotta elettrochimicamente: uso dell'acetonitrile anione come attivatore dello zolfo elementare nella sintesi di tioammidi

Principal investigator: M. Feroci

13 000 Euro

Dispositivo di scansione multimodale per sistemi portatili per l'analisi di Beni Culturali

Principal investigator: G. E. Gigante

10 900 Euro

Mathematical Models and Controllability

Principal investigator: P. Loreti

9 000 Euro

Advanced beam position monitors for the Compton Gamma Source of the Extreme Light Infrastructure

Principal investigator: A. Mostacci

38 600 Euro

Engineered magnetic nanoparticles for bio-related applications: modeling, fabrication, characterization and testing

Principal investigator: M. Rossi

15 000 Euro

Fast Monte-Carlo platform development for rapid Treatment Planning System verification and dose deposition monitoring in proton therapy

Principal investigator: A. Schiavi

15 000 Euro

Problemi non lineari sui frattali

Principal investigator: M. A. Vivaldi

13 000 Euro

## 2017 Large size projects

Non linear PDEs in geometry and physics

Principal investigator: A. Pistoia

53 750 Euro

## 2017 Medium size projects

Liquidi ionici di-cationici per applicazioni in chimica organica e in elettronica organica: sintesi, caratterizzazione e studi elettrochimici

Principal investigator: I. Chiarotto

35 750 Euro

Strutture algebro-geometriche e combinatori relative a grafi, quiver, Grassmanniane, codici e polinomi ortogonali.

Principal investigator: S. Capparelli  
12 000 Euro

Evolution phenomena in heterogeneous environments: application to biological systems, pedestrian motion and materials with memory  
Principal investigator: E. N. M. Cirillo  
13 300 Euro

Studio e caratterizzazione di nuovi elettrodi alternativi per le batterie litio-aria  
Principal investigator: A. Dell'Era  
13 300 Euro

Boundary Value Problems with Integrodifferential Terms on Fractafolds  
Principal investigator: M. R. Lancia  
12 255 Euro

Equazioni con diffusione nonlineare di tipo degenerare, singolare ed anomala  
Principal investigator: T. Leonori  
13 300 Euro

Optical 3D Metamaterial: optothermal material properties  
Principal investigator: R. Li Voti  
13 300 Euro

Beam energy measurement in advanced linear particle accelerators for electrons  
Principal investigator: A. Mostacci  
13 300 Euro

## Research and Professional Services (*Conto Terzi*)

Department personnel also performed research and professional services on behalf of private and public organizations, for an approximate income of 2 270 000 Euro in the period 2015–2017.



# Publications



## Journal Articles - Year 2015

1. L. Agosta, G. Zollo, C. Arcangeli, F. Buonocore, F. Gala and M. Celino, “*Water driven adsorption of amino acids on the (101) anatase TiO<sub>2</sub> surface: An ab initio study*”, *Physical Chemistry Chemical Physics* **17** (2015) 1556-1561
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26. S. Carillo, “*Erratum to: Some remarks on materials with memory: Heat conduction and viscoelasticity (Journal of Nonlinear Mathematical Physics 12(1), 2005)*”, *Journal of Nonlinear Mathematical Physics* **22** (2015) i-iii
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33. G. Cerulli Irelli and M. Lanini, “*Degenerate Flag Varieties of Type A and C are Schubert Varieties*”, *International Mathematics Research Notices* **2015** (2015) 6353-6374
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37. M. Clapp, J. Faya and A. Pistoia, “Positive solutions to a supercritical elliptic problem that concentrate along a thin spherical hole”, *Journal d’Analyse Mathématique* **126** (2015) 341-357
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41. F. Collamati, A. Pepe, F. Bellini, V. Bocci, G. Chiodi, M. Cremonesi, E. De Lucia, M.E. Ferrari, P.M. Frallicciardi, C.M. Grana, M. Marafini, I. Mattei, S. Morganti, V. Patera, L. Piersanti, L. Recchia, A. Russomando, A. Sarti, A. Sciubba, M. Senzacqua, E. Solfaroli Camillocci, C. Voena, D. Pinci and R. Faccini, “Toward Radioguided Surgery with  $\beta$ -Decays: Uptake of a Somatostatin Analogue, DOTATOC, in Meningioma and High-Grade Glioma”, *Journal of Nuclear Medicine* **56** (2015) 3-8
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