Francesco Tavanti

Computational Modeling of Protein-Nanoparticle Interactions

Interest in Nanoparticles (NPs) is growing due to their unique physical, chemical, electro-magnetic and optical properties. These unique properties are given mainly by the high surface-volume ratio that confers to them a very active surface. Moreover, NPs are small enough (typically their diameter less than 100nm) to interact with cell machineries and to reach inaccessible body parts, such as the brain.
Therefore, an increasing number of applications of NPs is emerging in nanomedicine, drug delivery and imaging, in nanotechnology and in nanotoxicology.
However, the determinants for the interactions with biological systems are relatively unknown since, when NPs are exposed to the biological medium, they are immediately covered with biomolecules, such as proteins, forming a "bio-corona". This confers a new biological identity to the NPs and determines the subsequent cellular/tissue response.
Notwithstanding the recognized importance of computational simulations to help understanding the interaction of NPs with living systems,[1,2] only a few computational works are present in the literature. These studies, in fact, still constitute a very challenging goal since they require integration of multiple hierarchies of models, each differing in several orders of magnitude in terms of scale and properties [3,4].
I will start my research project on the study of protein-(Au, Ag)NPs interactions by using Coarse Grained (CG) models. The CG method consists in the reduction of the number of degrees of freedom by condensing a group of atoms in a single interactive site (bead). In this way, by saving computational cost, it will be possible to simulate the process of bio-corona formation. Several models for the Au and Ag NPs will be tested. The proteins will be initially treated with a single bead model where each amino acid is replaced by one bead centered on the alfa-carbon (Cα) position. In this manner, the secondary structure of the proteins is unaltered. This simple CG model initially used will be successively refined and the details of the interactions will be studied with an all-atom model, which has good spatial and temporal resolution.
In order to validate the computational procedure adopted, two proteins, apolipoprotein and ubiquitin, will be first investigated since experimental data (bio-corona dimensions, number of interacting proteins, protein interaction sites, change in the secondary structure upon protein interaction) for their interactions with Au and Ag NPs are available in literature.
Once validate, the computational approach will be used to study how physico-chemical properties properly-tailored to meet specific application requirements are affected by the core, corona and interface of the NPs.

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Giorgia Ferrari

Analytical characterization of the introduction of new technologies for ceramic glazing and decoration

During the last 6-7 years the ink-jet digital decoration of ceramic tiles has shown a huge development. This led to a necessary technological adjustment of digital printers and, above all, of inks.
The aim of this research is the chemical-physical characterization of inks in commerce nowadays, and the reformulation of their components and production processes to improve their performances.
We will apply FTIR, XRF, micro-Raman, TGA-DTA, GC-MS, ICP-MS, granulometric and viscosimetric analysis to find the best materials (pigments and carriers) for inks, to study their behavior under physical stress, the pigments chromatic output and inks polluting emissions during combustion.
This project will be carried out in collaboration with Italian ceramic factories, research institutes and chemical laboratories, as well as foreign and Italian factories which produce printers and inks.

Dario Iori

Ecological functions of secondary metabolites isolated from polychaetes

Secondary metabolites are now believed to be at the basis of ecological specialization because they serve as protection against “enemies” (predators, competitors, parasites). In marine organisms, most secondary metabolites have been isolated from sponges, ascidians, soft corals, seaweeds, marine microbes. In polychaetes, a large group of aquatic invertebrates that colonize all marine environments, the occurrence of chemical defences was demonstrated only in few species.
The overall aim of my 3-years PhD research will be to assess the occurrence, ecological significance and role in chemical defences of secondary metabolites extracted from Mediterranean polychaetes. Worm species will be selected in order to obtain a representative sample of the polychaetes functional and systematic diversity.
For each chosen species, several research activity will be performed:
1) sampling/acquisition of worms and their maintenance in aquaria;
2) assessment of rough exudates toxicity by bioassays and palatability tests;
3) sequential extraction of secondary metabolites from worms’ body and exudates with organic solvents and extract evaporation;
4) assessment of evaporated rough extracts toxicity and palatability
If the research activity 2 or 4 will evidence toxicity and/or unpalatability, the active rough extracts will be characterized by LCMSIT. Then:
5) the active rough extracts will be purified and fractionated by chromatography;
6) each fraction will be evaporated and analyzed by LCMSIT;
7) the appropriate purified fractions will be used for ecotoxicological and palatability tests;
8) the toxic/unpalatable fractions will be further analyzed by NMR spectroscopy and elemental analyses in order to achieve the chemical structure of the active compound.
The study has the aim to improve our knowledge about chemical defences of polychaetes; it will also lead to the isolation and purification of molecules with potential application purposes.

Silvia Barbi

Optical and mechanical properties of glasses containing rare earth

Rare earth (RE) containing glasses have been largely investigated in the recent past due to the peculiar properties that the rare earth element adds to the materials properties. During this PhD the interest will be focused on glasses in which the RE promote optical and mechanical performances that could found application in two recent fields such as dental and photonic applications. For the first application the mechanical properties will be optimized in terms of impact and wear resistance, flexural strength. Moreover high density and higher biocompatibility will be promoted by ad hoc design of the glass compositions. For the second application RE will be added to the glass matrix to promote optical properties such as colouration and/or photoluminescence. RE containing glasses and glass-ceramics will be designed and optimized by using the DoE (Design of Experiment) approach to study systematically the formulations in order to achieve strong improvement in the final response. This could open to potential technological applications of the materials that will be explored during the research project.

Valentina Nicolini

Investigation about structure and chemical and biological proprieties of bioceramics doped with Cerium oxide

Cerium oxide has been proved to exhibit strong antioxidant proprieties [1-2], due to the equilibrium Ce^{3+}/Ce^{4+}. This capacity makes Cerium oxide able to protect the cells from the oxidative stress caused by the reactive oxygen species (ROS), such as superoxide radical. In fact Ce^{3+}/Ce^{4+} -containing system present a mimic SOD activity [3]. Thus, our aim is to synthesize, via sol-gel and via melting, bioglasses doped with different percentage of CeO_2 and to study their behavior once that they are placed in an environment rich in ROS. At the same time, we plan to study the structure of these glasses, using computational techniques.
To reach our purpose, we plan to make tests in H_2O_2 and in SBF, and to do instrumental analysis, such as: XPS, SEM, TEM, XRD, ICP, UV-VIS and NMR. Furthermore, we intend to study the behavior of the bioglasses doped with CeO_2 at different pH.
The collaborations expected are with the group of “Computational Chemistry” (Prof. M.C. Menziani, Dott. A. Pedone) of the Department of Chemical and Geological Sciences, regarding the structures of our glasses, and with the group of “Physics of Nanomaterials” (Prof. S. Valeri, Dott. P. Luches) of the Department of Physical, Informatics and Mathematical Sciences, concerning XPS analysis and tests of deposition of CNPs on the surfaces of our glasses.

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Cecilia Salocchi

Methane derived carbonates: markers of the evolution of Epiligurian and foredeep successions in the Northern Apennine (Miocene)

Methane-derived authigenic carbonate in the northern Apennines represent fossil exemples of seepage related to emissions of hydrocarbon-rich fluids.
Mechanisms that can trigger submarine seepage of methane-dominated hydrocarbons are :
1. tectonic events (tectonics constrains the plumbing system, with faults and fractures serving as conduits and channelling water and methane up to the seafloor);
2. climatic events (carbonate formation seems to correlate with cold periods and sea-level low-stand).
In this project peculiar methane-derived carbonates of Miocene age in the Emilia-Romagna Apennine are studied using a stratigraphic, petrographic and geochemical approach. Carbonates will be used to detect factors (climatic, eustatic, tectonic) controlling sedimentation and evolution of the Epiligurian Miocene shelf carbonates and their relation with adjacent foreland basins.

Manuela Deiana

Influence of groundwater flow on space and time evolution of rock-slide.

The aim of the research is to define groundwater processes (infiltration, sub-surface flow-path) and their effects on space and time evolution (short and long term) of deep-seated rock – slide located in the northern Apennines of Italy. The study sites are: the Berceto landslide (Parma Province), the Pietra di Bismantova, the Montecagno and the Collagna landslides (Reggio Emilia Province).
In order to understand groundwater infiltration processes, to define infiltration area, to quantify its travel time within the landslide body, and to recognize groundwater flow-paths the research will consist of:
-Hydrogeological characterization of landslide materials (permeability K, storativity S);
-Groundwater sampling (from springs, piezometers and rivers);
-Hydrochemical investigations (definition of physical parameters and chemical analysis);
-Groundwater stable and radiogenic isotope investigations (δ18O, δ2H, δ3H and 87Sr/86Sr);
-Collecting of meteorological data;
-Tracing test by means of isotopes and/or saline solutions;
-Hydrogeological and Hydromechanical 3D finite elements modeling (realized in collaboration with the Laboratory of Soil Mechanics, EPFL, Lausanne-Swiss);
In order to understand the influence of groundwater flow on landslide space and time evolution, the research will be carry out as follows:
-Monitoring of nowadays surface and deep deformations (through inclinometers and topographic benchmarks);
-Dating of landslide evolution by means of isotope investigations on the solid matrix (10Be,26Al,36Cl,14C).
The innovative approach of the research regards the contemporary use of isotope surveys to investigate both rock phase and water within landslide phenomena. Isotope investigations and analysis will be realized through the collaboration with IGG-CNR Pisa (IT) and the Universities of Delft (NL) and Liverpool (UK).

Andrea Bertolini

Realization of high-resolution gridded precipitation data set for the study of the effects of extreme events on slopes instability

The present project is aimed at the realization of a high-resolution gridded data set (1km x 1km) of monthly precipitations expressed in absolute values referred to Northern Italy.
Locally, where the data availability is sufficient, we will try to increase the temporal resolution of the data set, necessary to perform the analysis of precipitation extreme events and their effects on the instability of slopes.
The approach that will be used assumes that the spatio-temporal structure of the meteorological variable over a given area can be described in terms of the superimposition of two fields: the normal values related to a standard time period (e.g. 1961-1990), i.e., climatologies, and the deviations from them, i.e., anomalies.
The information coming from the spatial distribution of the normal values will be combined with those coming from the spatio-temporal behavior of the anomalies, to obtain a high-resolution grid of precipitation series in absolute values for the target area. Absolute values will be simply obtained by multiplying (precipitation anomalies are defined as ratios to the mean) the two fields (climatologies and anomalies).
Thanks to the availability of pressure and geopotential height fields, both reconstructed and forecasted (Regional Climate Models), together with the used of regressive models able to quantify and take advantage of the relation between predictors (atmospheric circulation pattern) and predicands (high resolution grid about precipitation expressed in absolute values), we will be able to extend, both in the past and in the future, the meteorological variable evolution, preserving the maximum spatial definition.
This high resolution meteo-climatic reconstruction/prediction will be used to analyze the extreme events and their effects on slope instability in selected areas, e.g. Eastern Liguria and Trentino-Alto Adige.

Matteo Ruocco

Census of Emilia-Romagna's (Italy) ponds: location and ecological characterization of different typologies for their management and conservation

Ponds are defined as temporary or permanent standing water body between 1 m2 and 5 hectares in surface area (European Pond Conservation Network, EPCN, 2008). They are located in a wide range of habitat typologies: from the sea level up to the alpine area. Important for the role they play in maintaining freshwater biodiversity, ponds have a high ecological value because of the flora and fauna they support: with many protected species which are threatened at both national and international levels. Furthermore, ponds are recognized as stepping stones habitats from the "Habitat" Directive (92/43/CEE) as they play an important role in providing connectivity across landscapes. Finally, these water bodies have high scientific and educational value and they are often important form a socio-economic point of view.

The aim of the present research is to locate the ponds of Emilia-Romagna: an Italian region located in the northern part of the country. A quick evaluation of the conservation status of the ponds will be carried out and the collected data will be insert in an international inventory: Pan Mediterranean Wetlands Inventory (PMWI). Important Areas for Ponds (IAP; EPCN, 2010) will be identified following the criteria proposed by the EPCN in order to recognize areas that are important for biodiversity and to raise awareness about these habitats. A complete study on some of the most interesting habitats will be achieved with floristic inventories, vertebrates and macro-invertebrates census and the monitoring of the main chemical-physic characteristic of the water.

Results will be useful for the knowledge, the management and the conservation of such threatened habitats which are still not properly protect in the study area.