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PhD Yearbook | 2010

Chair:
Prof. Carlo Bottani

DOCTORAL PROGRAM IN RADIATION SCIENCE AND TECHNOLOGY

The thesis works that are presented in this Yearbook are very representative of the multi-disciplinary research activity performed within the context of the PhD educational and research program in Radiation Science and Technology (RST). The latter is specifically designed to provide the student with the state-of-the-art in a wide range of research fields related to the application of nuclear and non-ionizing radiations, to foster the growth and strengthening of research skills in our young researchers, to fully integrate their efforts made by our young researchers within the research performed in our Department of Energy, which is aimed both at obtaining basic results in RST through innovative instrumentation and methods, and at developing and testing effective technological solutions for specific applications. In the last decades the research activity was mainly devoted to:

- Planning and development, by means of analytical-numerical methods, empirical models, and experimental studies, of innovative nuclear plants for energy conversion, aerospace, and fusion applications.
- Methods of safety and reliability analysis applied to the design and diagnostic of nuclear systems, and in general of high risk environments.
- Radio-protection for environmental monitoring, nuclear plants decommissioning, radioactive waste disposal, underground dispersion of contaminants.
- Development of innovative high-performance radiation detectors, and their applications to R&D fields such as space science, synchrotron radiation, high-energy physics, or to topics of interest for the large community such as medical investigations, cultural heritage preservation, environmental monitoring, nuclear safety.
- Synthesis by ionic implantation or pulsed laser ablation of innovative materials, such as nanostructures and "soft" materials, and their structural characterization by radiation scattering techniques (Raman, Brillouin, X-ray, neutron, and quasi-elastic light scattering), or tunnel/atomic force microscopy.

Starting with the new 25-th doctoral cycle (2010) this doctoral program and the Energy doctoral program are unified in the new Energy and Nuclear Science and Technology doctoral program.

For what concerns the specific thesis works presented in what follows, Stefano Buzzaccaro investigated systems of colloidal particles interacting via very short-ranged attractive forces and obtained valuable and often unforeseen insights on the contingency of the liquid state and on the origin of metastable gel or glassy phases with relevant potential applications in the fields of crystallization and competitive adsorption of proteins, percolation in microemulsions, flocculation and renneting. Valentino Di Marcello developed a multi-physics approach to the modelling and analysis of nuclear reactor core behaviour and applied it to the study of the dynamics of Molten Salt Reactors (MSR). In the last years, this kind of nuclear reactors has been the subject of a growing and renewed interest from the scientific community in the framework of the Generation IV International Forum. The thesis work of Fabio Donati focused on the development of new Scanning Tunneling Microscopy and Spectroscopy (STM and STS) tools (both theoretical and experimental) and on their application in the investigation of magnetic surfaces. Spin polarized STM (the technique used in this work in an innovative way) is a very hot topic in both surface physics and nanotechnology. Paolo Ferrari worked in the field of organ dose conversion coefficients for neutrons and photons, investigated with voxel (3D) models and Monte Carlo simulations and validated through the irradiation of complex anthropomorphic phantoms. He obtained useful results in view of radiotherapy applications. The thesis work of Vito Memoli dealt with the modeling, again based on the multiphysics approach, of three different innovative nuclear reactors. In particular, the developed models are aimed at performing both static and dynamic analyses of reactor core. The three systems considered in this work are the space reactor SURE, the Lead cooled Fast Reactor and the Molten Salt Reactor. All these systems cannot rely on previous experience and require a major effort in terms of system modeling and simulation. Nicola Pedroni developed advanced Monte Carlo simulation methods and neural network regression for the reliability analysis of nuclear passive systems. The methods have been tested on a case study involving the natural convection cooling in a Gas-cooled Fast Reactor after a Loss of Coolant Accident. Giovanni Sansavini analyzed critical infrastructures with respect to their vulnerabilities to random failures and targeted attacks. Critical infrastructures are large scale, spatially distributed, complex systems which provide vital services for modern society, such as energy supply, transportation, information and telecommunication, drinking water distribution, including wastewater treatment. The work of Daniele Vigolo had the purpose of investigating nonequilibrium effects arising in "complex fluids" (nanometer-size latex particles, surfactant micelles or polymer suspensions) in the presence of thermal gradients. A successful application of thermophoresis as a microfluidic separator was also tested.

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DEPLETION FORCES IN SURFACTANT-COLLOID MIXTURES

Stefano Buzzaccaro

An important distinction between conventional or "simple" liquids and solids is that the former quickly take the shape of the container in which they are kept, while the latter maintain their shape indefinitely. Almost all "complex fluids'' are intermediate between solid and a liquid: while they maintain they shape for some time, they eventually flow. They are solids on a short time scale and liquids at long times: they are *viscoelastic*. Clearly, this rough definition is connected to a human time scale through the designation "for some time". Nevertheless it does make sense to define a class of materials based upon their ability to flow or not during a (human) experiments. Examples of such "complex liquids" are everywhere: *polymers, paints, (micro-)emulsions, surfactant solutions, biological fluids, milk*. It is evident that their study has myriad of applications and interests a billion dollar market. A distinguishing feature of complex fluids compared to ordinary condensed matter is that there always is a length scale involved that is large with respect to the size of individual atoms and molecules. This separation of length scales makes it possible to integrate out many degrees of freedom and give a more simplified description of the problem. A concise but meaning definition present in literature called them "Big Atoms". Colloidal particles dispersed in a medium encompass a large class of complex fluids. They are "solution'' of one phase of matter (solid, liquid, gas), the colloidal particle, into another that acts as the continuous phase (liquid, gas). Now, let us focus on solid particles dispersion. In this system the addition of other smaller components as polymers, salt, surfactant molecules that can auto-aggregate forming micelles, induce effective interactions between the bigger solid particles. This ability of easily tuning particles interaction has made colloidal dispersion one of the most useful experimental system in order to prove liquid state theories. In add, this particles are large enough to interact with visible light: Many convenient techniques are therefore applicable, particularly optical microscopy and light scattering, and investigations do not require the more difficult and expensive methods of electron microscopy, X-ray and neutron scattering**.** In this field the investigation of systems of colloidal particles interacting via very short-ranged (much smaller than particle radius) attractive forces has yielded valuable and often unforeseen insights on the contingency of the liquid state and on the origin of metastable gel or glassy phases. In this regard, the Adhesive Hard Spheres (AHS) limit, corresponding to an attractive potential of vanishing range has become the paragon model in the investigation of many topics, such as crystallization and competitive adsorption of proteins, percolation in microemulsions, even flocculation and renneting in dairy practice. Yet, to what extent real systems *quantitatively* conform to the simple AHS model is often scarcely scrutinized. A particular kind of short range attractive interactions largely studied in colloidal science are the **DEPLETION FORCES,** that kind of interactions induced by the addition into the colloidal suspension of *small* (here small "much smaller than particles size") non adsorbing components (polymers, micelles, spheres,...). When two big particles approach until the center-to-center distance is smaller than the typical size of the added component, this will be ejected from the overlap volume. The pressure unbalance generates a net attraction between the bigparticles. Depletion effects are commonly induced by adding to a colloidal suspension non-adsorbing polymers. An alternative route consists in using as a depletion agent the micellar aggregates spontaneously formed by a surfactant additive. In the first part of my PhD (Ch. 4, 5, 6) I investigate a system of AHS, in which interactions are induced by the addition of a non ionic surfactant. To do this it was natural to choice the easier depletion mechanism: micelles behave as an ideal gas and do not interact. To do this I exploit the fact that an accurate quantitative study of sedimentation profiles offers an excellent opportunity to obtain the full equation of state of the system (Ch. 4 and 7), hydrodynamic interactions (Ch. 5) and to provide quantitative information on the mechanical properties of gel phases (Ch. 6). As yet stated, interactions in colloidal suspensions can be easily tuned changing macroscopic properties of the system (temperature, micelles size and concentration, amount of salt,...). The capacity of controlling interactions is of fundamental importance to create new smart materials, i.e. photonic crystals. Most theoretical efforts have been devoted to study "ideal depletion", where depletant self-interactions are absents. A noticeable exception is the analysis of Hard Sphere binary mixtures. In Ch. 4, however, I will show that, even when depletant self-interactions are negligible at the level of the second virial coefficient they can still have rather important effects on the phase diagram. This opens up a totally new question, which I could summarize as follows: *what is the behavior of a colloidal suspensions in an effective solvent, made of a solution of much smaller colloids which have a generic self-interactions?*. This question is strongly linked to some other problems in colloid physics which have been extensively addresses in the last few years: for instance, *what is the behavior of colloids in a "structured" solvent, such as a simple binary mixture close to a critical point or in a liquid crystal?* From the theoretical point of view, this amounts to investigate whether the classical McMillan-Mayer approach to the potential of the mean force can be extended to yield general ideas on the phase behavior of mesoscopic particles in such a structured solvent. Sticking to depletion interactions, the problem is far from being trivial. Consider for instance only repulsive self-interactions of the depletant. On the one hand, its osmotic pressure increases, so that depletion forces on the colloids become stronger. On the other, however, the depletant gets structured, and this has been shown to reduce depletion. According to a metropolitan legend, at least for binary Hard Spheres, this second contribution eventually wins, so that depletion is weaker than in the ideal case. But the theoretical results have been grossly overlooked: When the repulsive self-interactions are longer range, as for electrostatic forces, the "osmotic" effect becomes even more dominant. In Ch. 7, indeed, I give ample evidence that depletion interactions using a charged depletant becomes much stronger, to the point that even a tiny amount of surfactant is sufficient to phase-separate the colloids. An even more interesting question concerns the effect of strong attractive forces between the depletant. Here the depletant osmotic pressure decreases, so that one should get weaker depletion. But structuring effects play a strongly conflicting role, increasing in this case depletion forces. As it is well known, the surfactant micelles of a non ionic surfactant, which at room temperature behave almost as an ideal gas, show an inverted consolution curve with water at high (but accessible) T. In Ch. 8 I demonstrate that if one then add colloids, the amount of surfactant needed to phase-separate strongly decrease by increasing T and approaching the surfactant-water consolution curve: this trend is strongly correlated with the growth of the correlation length of the micellar solution. I show that this " links" depletion with experiments on **critical Casimir effects** (fluctuations between two macroscopic bodies can induce a force of attraction between them), giving the first quantitative experimental evidence of this effect in surfactant-colloid mixtures.

DEVELOPMENT OF A MULTI-PHYSICS APPROACH TO THE MODELLING AND ANALYSIS OF MOLTEN SALT REACTORS

Valentino Di Marcello

In the present PhD thesis, a multi-physics approach to the modelling and analysis of nuclear reactor core behaviour was developed, and applied to the study of the dynamics of Molten Salt Reactors (MSR). In the last years, this kind of nuclear reactors has been the subject of a growing and renewed interest from the scientific community in the framework of the Generation IV International Forum. The Multi-Physics Modelling (MPM) approach was implemented in the unified simulation environment offered by the finite element COMSOL Multiphysics® software. It resulted able to properly catch the synergy between the different phenomena involved in the reactor core behaviour, whose modelling would otherwise require either the adoption of dedicated simulation tools (with drastic modifications of their structure) or the development of *ad hoc* numerical codes for the particular analysed situation. The Molten Salt Breeder Reactor (MSBR) developed at the Oak Ridge National Laboratory during the 60s was chosen as reference configuration for the analyses. In such kind of circulating fuel reactor, like the other MSRs, the coupling between neutronics and thermo-hydrodynamics is a key issue. This feature cannot be neglected in order to perform an adequate description of the reactor dynamic behaviour, which shows peculiar aspects with respect to solid-fuelled conventional nuclear power plants. The developed MPM methodology and the adopted models for neutronics and thermo-hydrodynamics have required a deep investigation for what concerns the assessment and the extension of the COMSOL simulation environment.

As far as thermo-hydrodynamics is concerned, a generalized analytic approach was developed and exploited for the assessment of COMSOL simulations, making also use of a dedicated finite volume computational fluid dynamics code (FLUENT®), in order to better appreciate the differences in numerical approaches to turbulence. The analytic approach was built in order to carefully take into account the molten salt mixture specificities (i.e., a fuel that operates also as coolant), the reactor core power conditions and the heat transfer in graphite. In this context, a Nusselt number correlation was developed, which takes into account the effect of internal heat generation on fluid heat transfer characteristics.

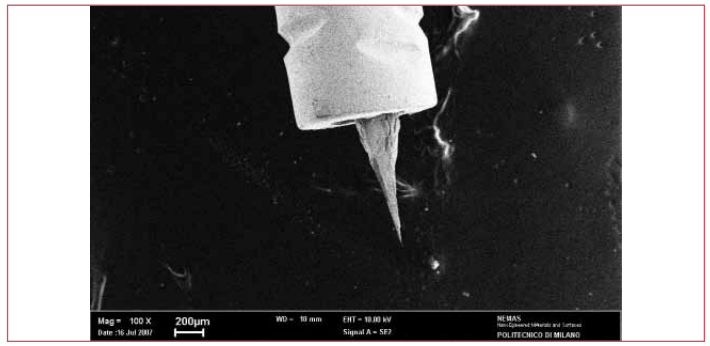
As far as neutronics is concerned, a module for the "reactor physics" was built in the COMSOL environment of simulation, and allowed to extend the potentialities of this software. Numerical results were assessed by means of: i) a code-to-code comparison with dedicated neutron transport codes, in the case of static fuel; ii) a comparison with a simplified neutron kinetics model, which resulted representative of the zero-power dynamics of the Molten Salt Reactor Experiment (thanks to the availability of experimental data), in the case of circulating fuel.

After the assessment of the COMSOL capabilities to cope with the adopted models for the neutronics and the thermo-hydrodynamics, the MPM approach was applied to study the dynamic behaviour of a single-channel representative of the average conditions of the MSBR core. Several different transients were analysed, such as those driven by: reactivity variations due to control rod movements; fuel mass flow rate variations due to the changing pumping rate; presence of periodic perturbations, due to local precipitation of fissile solid compounds within the molten salt mixture. The analyses gave significant information on the MSBR dynamic behaviour and highlighted the several advantages and potentialities offered by the proposed MPM approach (for instance, the "modularity", namely the possibility to include other physical phenomena and couplings). These potentialities are of more general interest in the prospect of studying the design configuration of next generation MSRs.

DEVELOPMENT OF SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY TECHNIQUES FOR THE INVESTIGATION OF MAGNETIC SURFACES

Fabio Donati

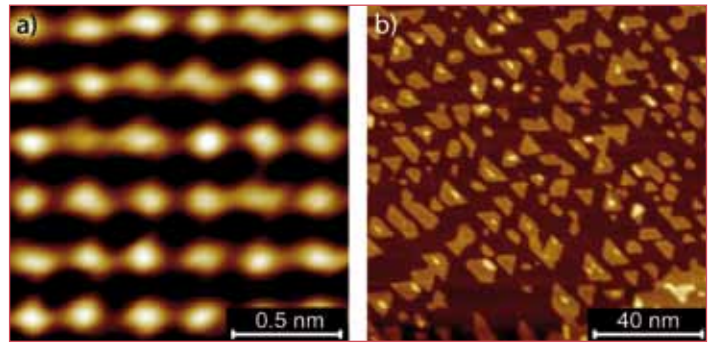
Scanning Tunneling Microscopy (STM) is a probe imaging technique. By means of a tip that scans over a surface at a sub-nanometric distance, a tunneling current is generated when a bias voltage is applied. Since the tunneling current behaves exponentially with respect to the distance between the tip and the sample, the effective interaction area is reduced to a few atoms of the tip, allowing to reach the atomic resolution. The extremely high achievable resolution is widely exploited in the investigation of surfaces and nanostructured systems and STM is now universally recognized as a fundamental tool for the investigation of surfaces on the nanometric scale. The tunneling current depends on the tip and sample electronic structures, thus allowing the possibility of acquiring local information about surface electronic properties.
In particular, by measuring the tunneling current with respect to the applied voltage, this technique can be used also to perform the so-called Scanning Tunneling Spectroscopy (STS). STS can provide information about the electronic local density of states (LDOS) with extremely high spatial resolution. However, the connection between experimental data and the physical quantities of interest is not straightforward and specific models are needed in order to properly interpret raw STS information.



1. Electron microscope image of a Cr bulk tip

STM can also be used to investigate magnetic properties of surfaces by means of magnetic tips (Spin Polarized Scanning Tunneling Microscopy/ Spectroscopy, SP-STM/SP-STS). Exploiting the dependence of the tunneling current on the relative orientations of tip and sample magnetizations, it is possible to map the magnetic domains of surfaces. Since the sensitivity to the surface magnetic properties is achievable only using magnetic tips, one of the most delicate issue is to produce STM tips with reliable and stable magnetization behavior.
Among the great number of systems which can be investigated with STM/STS and SP-STM/STS, the case of low-dimensional magnetic systems (e.g. surfaces and supported clusters) is particularly interesting. The investigation of such systems is motivated by the growing interest in magnetic junctions-based devices and by the need of reducing the dimension of the single bit in data storage applications. The knowledge of the electronic and magnetic properties of the matter at the nanoscale might provide the key for developing novel materials and structures for high performance devices.

This thesis work have been focused on the development of new STM and STS tools (both theoretical and experimental) and on their application in the investigation of magnetic surfaces. First, the important issue of modeling the tunneling process for the interpretation of STS data has been considered. Depending on the theoretical framework, two possible approaches to the description of the tunneling process have been developed. In the framework of the Wentzel-Kramer-Brillouin approximation, several improvements of the actual theory have been proposed. They have been tested by means of simulated *dI/dV* curves based on model sample and tip LDOS and used in interpreting experimental data taken on the Au(111) and the Si(111)-7×7 surfaces. With the aim of improving the description of the tunneling process, we have developed a full 3D analytical model of tunneling in the framework of the Transfer Hamiltonian theory. In this way, fundamental aspects like the sample surface band structure and the symmetry of the tip states have been included. We have then applied both the model to the case of Shockley states.



2. a) Atomic resolved STM image of the Fe(001)-p(1x1)O surface. b) Fe islands deposited on Au(111)

Another line of this work has concerned with the development of experimental techniques for SP-STM/SP-STS. We have developed a novel method for producing bulk Cr tips (Fig. 1). These tips have been first characterized onto non-magnetic surfaces like Au(111) and Si(111)-7×7. Characterizations of the magnetic behavior of these tips have been performed both at RT and at 8 K in the presence of magnetic field. RT measurements on Cr(001) surface have shown that the tip is capable of detecting SP signals from different domains of the surface with an in-plane magnetization. LT measures on Co/Cu(111) have shown that, despite its expected antiferromagnetic character, tip magnetization is sensitive to the presence of an external magnetic field.

The third part of this work has been devoted to the application of the developed methods to the investigation of magnetic surfaces. Both the Fe(001)-p(1×1)O surface and the Fe/Au(111) system have been investigated. For the Fe(001)-p(1×1)O surface, we have performed a structural characterization down to the atomic scale. By comparing the STM images with DFT calculations, we conclude that oxygen atoms are mainly probed when the tip is scanned at high setpoint current (Fig 2a), while Fe atoms are instead visible for low setpoint current. STS measurements have been performed to study the LDOS of the surface. We have finally investigated the Fe/Au(111) system. In this case we first focussed on its growth characteristics up to the coalescence regime. The coalescence of monoatomic islands has been observed to start at about the same coverage of 0.35 ML (Fig 2b). STS performed with W and Cr tips down to 25 K onto Fe islands have allowed us to identify a pronounced peak in the surface DOS, located at 50 meV below the Fermi energy. Similarly to what observed with Co/Au(111) and Cr/Au(111), this can be interpreted as a feature of the d states of Fe. The position of this peak has been found to shift to higher energy moving from the center to the periphery of the islands.

ORGAN DOSE CONVERSION COEFFICIENTS, FOR NEUTRONS AND PHOTONS, INVESTIGATED WITH VOXEL MODELS AND MONTE CARLO SIMULATIONS AND VALIDATED THROUGH THE IRRADIATION OF COMPLEX ANTHROPOMORPHIC PHANTOMS

Paolo Ferrari

Ionizing radiations are employed in medical, industrial and research applications. In this field the absorbed dose, that is, at first approximation, the energy released by the radiation traversing a certain volume of body tissues divided by its mass, is the quantity to be evaluated. The absorbed dose is difficult to be estimated. In some medical practices, radiation detectors can be introduced in the body through catheters but normally the dose estimates are based on the application of conversion coefficients that allow coupling a measurable quantity of the radiation field (kerma in air, dose to the air, particle fluence) to the absorbed dose in the body organs. These conversion coefficients can only be evaluated employing computer codes, simulating the radiation transport, and anthropomorphic numerical models reproducing the radiation interactions in the body tissues. The official conversion coefficients are published by international radiation protection committees and are strictly valid only for personnel routine radiation protection purposes. The dose reconstruction in medical applications or in particular exposure scenarios requires *ad hoc* evaluations. In these cases validations through plastic phantoms and easy reproducible irradiation conditions are necessary to determine the level of accuracy of the calculated quantities.

In the present work the conversion coefficients for neutron and photon fields were investigated through the Monte Carlo code MCNPX applied to a new computational model representing an adult man whose characteristics are very similar to those defining the *reference man*. The *reference man*, introduced by International Commission on Radiological Protection in the sixties, represents the "average man" of the Western-Caucasian population in terms of distribution of volumes and masses of the body organs. The employed new computational model was obtained from the CT scan of a real plastic phantom, 175 cm height, containing the main organs and the skeleton. The phantom was made of PMMA and its different parts could be filled with water. Skeleton and lungs were made of polyethylene and polyurethane respectively. The CT image set of the plastic phantom was treated with imaging software and home-made C routines. The different parts of the body were defined through an automatic segmentation procedure, based on CT numbers, followed by a manual optimization of each CT slice. That procedure generated a 3-D matrix employed for the new computational model construction.

The validation of the couple of phantoms (plastic and computational one) was performed irradiating the plastic model and simulating the exposure scenarios with the computational one. Such procedure allowed determining the level of accuracy of the conversion coefficients afterward evaluated with the computational model.

The measurements in the plastic model required the characterization of proper sets of dosemeters: for photons, thermoluminescent dosemeters (TLD - LiF:Mg,Cu,P) were necessary, not being possible to use ionization chambers inside the plastic phantom for positioning problems; for neutrons, passive polyallyldiglycolcarbonate track detectors (CR-39) were chosen to estimate the dose due to the "fast" component (E > 200 keV) of the spectrum. The TLDs accuracy were established with a benchmark with a thimble ionization chamber in a water phantom and ^{60}Cobalt source, whilst the CR-39 were exposed in an irradiation hall to a ^{252}Californium spontaneous fission source. These procedures allowed determining the sensitivity of the employed dosemeters sets.

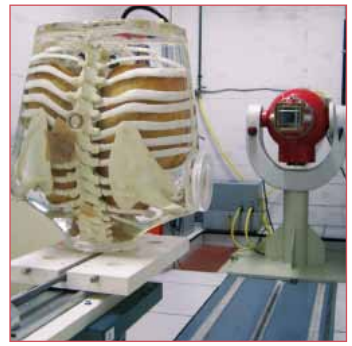
The validation procedure consisted in inserting TLDs inside the thorax of the plastic phantom and irradiating them to ^{60}Cobalt; the same was done for CR-39 with ^{252}Califronium neutron source. These two irradiation scenarios were replicated with the computational phantom. Monte Carlo evaluated quantities are expressed per source particle. In order to compare measurements and simulations, the previous dosemeter characterizations were replicated through MCNPX simulations. The obtained normalization factors were applied to the subsequent simulations with the anthropomorphic computational phantom.

During validation, for neutrons, the irradiation hall was modeled aiming at evaluating the radiation field component scattered from the walls, the ceiling and the floor (about 5% in the mid-plane axis but increasing at the back of the phantom due to the proximity of the nearest wall). The results of the validation showed a satisfactory agreement between measurements and simulations.

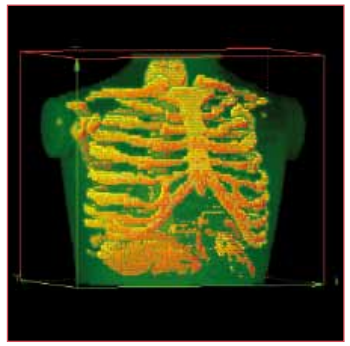
In the second part of the work, the validated computational model was employed to estimate organ dose conversion coefficients for parallel, aligned monoenergetic fields of photons and neutrons. The obtained conversion coefficients were compared with those calculated with other models, derived from real human CT and published in the recent literature. The good agreement demonstrated the quality of the new model and the possibility of assuming the calculated values as representative for the human population. Indeed the possibility of using the two phantoms as a unique integrated tool, employing the plastic model for measurements and using the computational to estimate any correction factors, is an important feature of the developed system.

One of the main expected applications of this couple of models is the patient dosimetry. In "traditional" radiotherapy neutron dose evaluation is needed. Neutrons are produced by the head shielding material of the medical accelerator with energy higher than 12 MV. This dose cannot be evaluated with the conventional treatment planning and can be estimated only with proper measurements and numerical simulations.

The same problem rises with radiotherapy with carbon ions, as reported in recent literature. The proposed phantoms can be proficiently used in such estimates. Indeed the possibility to insert TLDs enriched in ^{6}Li coupled with CR-39 track detectors allows employing them also in reactor irradiation facilities that can be of interest for the dosimetric aspects of NCT and BNCT (Neutron and Boron Neutron Capture Therapy).



1. ^{60}Co plastic phantom thorax irradiation during validation procedure



2. An image of the thorax of the computational model

MODELING APPROACHES FOR ANALYSIS OF INNOVATIVE NUCLEAR REACTORS

Vito Memoli

This thesis work deals with the modeling, mainly based on the multiphysics approach, of three different innovative nuclear reactors. In particular, the developed models are aimed at performing both static and dynamic analyses of reactor core. The three systems considered in this work are the space reactor SURE, the Lead cooled Fast Reactor and the Molten Salt Reactor. The definition of a reactor model constitutes a very important phase in the design process, especially for innovative reactor layouts, which cannot rely on previous experience and require a major effort in terms of system modeling and simulation. Moreover, the developing of suitable control strategies to ensure reactor safety during all the reactor operation heavily depends on the adequacy of the reactor model. Generally, reactor models can be developed on the basis of either simple or complex geometries and physical assumptions. In some cases, point reactor models can give satisfactory results in terms of the overall reactor behavior. This is the case of the Space Reactor SURE, which, far from the real deployment, needed a preliminary analysis in order to evaluate its feasibility in terms of safety and viability. In particular, in order to improve these features, a new layout has been proposed, which (instead of PWR technology) provides a boiling water coolant driven across the core channels by a primary circulation pump, along with an innovative reactivity control system based on the regulation of the primary pump operating regime. The originality of such configuration for a space reactor (potentially rescalable to larger power for terrestrial Generation III+ applications) required a detailed neutronic analysis mainly aimed to the development of a dynamic model of the primary system, which accounts for the enhanced thermal hydraulics and neutronics coupling. The set up model was mainly oriented to the study of the behavior of the innovative RCS, which should guarantee the correct and safe reactor functioning during both operational transients and long-term reactivity variation due to fuel burn-up. The model was implemented in MATLAB/SIMULINK and permitted to demonstrate that a) the system power can be controlled during operational transient by regulating the pump rotation velocity, which can be done using a simple inverter; b) the long-term regulation of the pump mass flow rate allows the reactor to be run with no need of human intervention for a period of time as long as 7 years.

The peculiarity of the Molten Salt Reactor systems, characterized by a strong coupling between the fluid dynamics and neutronics, suggested using an advanced modeling technique represented by the multiphysics approach which, in the recent years, great effort has been spent for. Among the most versatile multiphysics tool, COMSOL has been chosen due to its full integration capabilities with MATLAB/SIMULINK environment, which represents a reliable instrument for dynamics and control analysis. The study of Molten Salt Reactor physics and the related model development was primarily aimed at the qualification of COMSOL as a valid nuclear engineering tool. Thus a simple geometry was adopted, whereas the physical modeling takes into account the turbulence phenomena adopting computational fluid dynamics scheme, like the Reynolds Averaged Navier Stokes (RANS) k-ε. As for the neutronics, since the MSBR is featured by a thermal spectrum, the two group diffusion theory was adopted. Besides the thermal hydraulic model, deeply studied, tested and validated at Politecnico di Milano, a crucial point concerned the neutronics modeling. More precisely, the multiphysics model needed the definition of a coupling scheme capable of taking into account in a heterogeneous way the effect of the temperature of both fuel salt and graphite (characterized by very different thermal time constants) on the neutron spectrum. Thus, a series of cell calculations have been performed with NEWT using ENDF/B-VI.7 library, in order to create a group constants database obtained by collapsing the 238 group library over the two regions of interest (graphite and fuel salt) for different values of fuel and graphite temperature. An interesting analysis regarded the study of accident transients featured by system periodic perturbations due to precipitation of fissile material, which was modeled by taking into account the space and time-variation of the cross sections of fuel region across which the precipitated fissile material is swept by the fuel velocity.

The same methodology developed for the Molten Salt Reactor was applied to the lead cooled fast reactor ELSY, a promising design to meet all the goals of Generation IV. Differently from the MSBR, ELSY is characterized by a weaker coupling between thermal hydraulics and neutronics, which means small temperature feedback on reactivity (Doppler and coolant temperature effect), as shown in the kinetic parameter calculation with the multiphysics single channel model. Being ELSY a fast system, more energy groups had to be taken into account in the neutron diffusion modeling in order to properly describe the fast neutron spectrum. As matter of fact, the major effort was spent for the two-dimensional core neutronics modeling implemented in COMSOL. The core model, which was compared with a more detailed 3-D neutronic model developed with ERANOS, returned acceptable results from the point of view of a preliminary analysis of the core performance and allowed to derive information about the main safety parameters. Finally, the coupling capabilities of COMSOL were exploited to develop a preliminary 3-D thermal hydraulic model of the core, which permitted to thermally characterize the core.

ADVANCED MONTE CARLO SIMULATION METHODS AND NEURAL NETWORK REGRESSION FOR THE RELIABILITY ANALYSIS OF NUCLEAR PASSIVE SYSTEMS

Nicola Pedroni

Modern nuclear reactor concepts make use of passive safety features, which do not need external input (especially energy) to operate and, thus, are expected to improve the safety of nuclear power plants because of simplicity and reduction of both human interactions and hardware failures.
However, the *aleatory* and *epistemic* uncertainties involved in the *functioning* and *modeling* of passive systems are usually larger than for active systems. Due to these uncertainties, the physical phenomena involved in the passive system functioning (e.g., natural circulation) might develop in such a way to lead the system to fail its function (e.g., decay heat removal): actually, deviations in the natural forces and in the conditions of the underlying physical principles from the expected ones can impair the function of the system itself even if i) safety margins are present and ii) no hardware failures occur.
In the analysis of such *functional failure* behavior, the passive system is modeled by a mechanistic code and the probability of failing to perform the required function is estimated based on a Monte Carlo (MC) sample of code runs which propagate the uncertainties in the model and numerical values of its parameters/variables.

In practice, the probability of functional failure of a passive system is very small (e.g., of the order of 10^{-4}), so that a large number of samples is necessary for acceptable estimation accuracy. Given that the time required for each run of the mechanistic code can be of the order of several hours, the MC Simulation (MCS)-based procedure typically requires considerable computational efforts.
In this thesis the computational burden associated to the analysis is tackled in two different ways: from one side, efficient sampling techniques are employed to perform robust estimations with a limited number of input samples drawn and associated low computational time; from the other side, fast-running, surrogate regression models (also called response surfaces or meta-models) are used to replace the long-running code in the passive system reliability analysis.

Advanced Monte Carlo Simulation methods

The use of two recent MCS methods, namely Subset Simulation (SS) and Line Sampling (LS) is investigated.
In the SS approach, the probability of the (*rare*) functional failure event is expressed as a product of conditional probabilities of some chosen intermediate and thus *more frequent* events. The problem of evaluating the *small* probability of functional failure is thus tackled by performing a *sequence* of simulations of *more frequent* events in their conditional probability spaces.
In the LS method, *lines* are used to probe the failure domain of the multi-dimensional problem under analysis. An "important direction" is optimally determined to point towards the failure domain of interest and a number of conditional, one-dimensional problems are solved along such direction, in place of the multi-dimensional problem.
Two main issues of the LS method are tackled in this thesis which are still under study for its practical application in reliability analysis:

1. LS relies on the accurate determination of the important direction, which requires *additional* runs of the system model.
2. LS has been shown to significantly reduce the variance of the failure probability estimator, but there is yet no indication that the number of samples drawn (and, thus, the number of model evaluations) can be reduced down to a *few tens* or *hundreds*, which may be needed in practical cases when computer codes require hours to run a single simulation.

This thesis addresses the first issue above by:

- comparing the efficiency of a number of methods proposed in the literature to identify the important direction;
- proposing a new technique to determine the important direction, based on the *minimization* of the variance of the LS failure probability estimator.
- With respect to the second issue above, this thesis aims at:
- assessing the performance of the LS method in the estimation of small failure probabilities (e.g., of the order of 10^{-4}) with a *very small* number of samples drawn (e.g., of the order of 5–50).

Empirical regression modeling

The construction of regression models entails running the code a predetermined, *reduced* number of times (e.g., 50-100) for specified values of the uncertain input variables and collecting the corresponding values of the output of interest; then, statistical techniques are employed for calibrating the internal *coefficients* of the regression model in order to fit the input/output data generated; finally, the long-running code is replaced by the regression model in the passive system reliability analysis: because calculations with the regression model can be performed quickly, the problem of long simulation times is circumvented.
In this thesis, the use of Artificial Neural Networks (ANNs) is investigated. In synthesis, ANNs are: i) '*learning*' statistical models inspired by the structure and functioning of the brain, ii) *universal* approximators of nonlinear functions and iii) structurally *redundant* and *fault tolerant* computing devices.

However, when using the approximation of the system output provided by an ANN model, an additional source of *model* uncertainty is introduced which needs to be evaluated, particularly in safety critical applications like those related to nuclear power plant technology. To this aim, we resort to *bootstrapped* regression models, i.e., ensembles of regression models. This allows quantifying, in terms of *confidence intervals*, the model uncertainty associated to the estimates provided by ANN models.

Conclusions

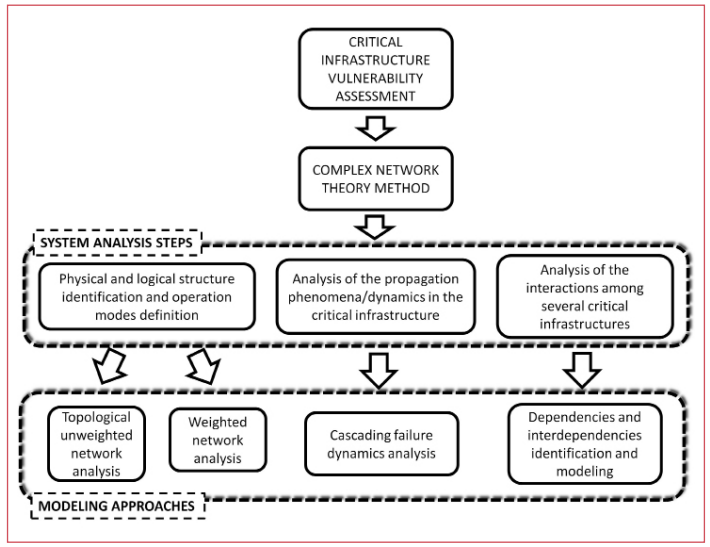
The above mentioned approaches and computational methods have been tested on a case study involving the natural convection cooling in a Gas-cooled Fast Reactor after a Loss of Coolant Accident.
On the basis of the results obtained, the following recommendations can be drawn for those analysts who approach the problem of passive systems reliability assessment:

a. If the analyst is *only* interested in the estimation of the failure probability of the passive system, the following procedure is suggested: **i)** determine the LS important direction by means of the *optimal* technique proposed in this thesis (based on the *minimization* of the variance of the LS failure probability estimator); **ii)** estimate the functional failure probability of the passive system by means of LS with a *small* number of samples (e.g., few tens).
b. This method is found to provide more accurate and precise estimates than standard MCS, Latin Hypercube Sampling and Importance Sampling (i.e., the methods currently used in Probabilistic Risk Assessment). However, notice that the LS technique allows *only* the calculation of the failure probability of the passive system, but it does not allow a *complete* uncertainty propagation: actually, no Cumulative Distribution Functions (CDFs) or percentiles of the code outputs of interest can be identified in a single simulation run.
c. If the analyst is interested in a more *complete* uncertainty propagation, two alternative options are suggested: **1.** the SS method offers a feasible means because it generates a *large* amount of samples by *sequential* simulations developed in the *whole* uncertain input space. On the other hand, different from the LS method, there does not seem to exist any indication that it is possible to reduce the number of code evaluations to below a few hundreds: as a consequence, if the code requires many hours, or days, to perform a single evaluation, SS is not suitable; **2.** in such cases, the use of fast-running ANN models instead of the long-running original code seems mandatory. However, the uncertainties associated to the ANN estimates *must* be quantified, e.g., by means of the bootstrap method. The use of ANNs is found to reduce the computational time by *several orders of magnitude*.

VULNERABILITY ANALYSIS OF CRITICAL INFRASTRUCTURES

Giovanni Sansavini

The subject of this PhD thesis is the analysis of critical infrastructures with respect to their vulnerabilities to random failures and targeted attacks. Critical infrastructures are large scale, spatially distributed, complex systems which provide vital services for modern society, such as energy supply (electricity, oil and gas supply as subsectors), transportation (by rail, road, air, shipping), information and telecommunication (such as the internet), drinking water distribution, including wastewater treatment.
From the standpoint of the recent developments in the field of complex systems theory and network analysis, there are two aspects which may allow gaining relevant insights on CIs, if properly analyzed: the study of the topology of the graph representing their structure and the study of their dynamic behavior through functional models reproducing the physical communication processes (mainly flow of some entity, such as electricity, data and vehicles) and the emerging propagation of failures taking place in it.
In this context, the goal of the PhD project here presented is to develop a methodology for critical infrastructure vulnerability assessment from the standpoint of complex systems theory.
The work has been performed at the Laboratorio di Analisi di Segnale ed Analisi di Rischio (LASAR, Laboratory of Signal Analysis and Risk analysis) of the Department of Energy of the Politecnico di Milano (http://lasar.cesnef.polimi.it/).



1. Pictorial view of the critical infrastructure vulnerability assessment presented in the current PhD research work carried out at LASAR

The conceptualization of critical infrastructure vulnerability assessment implies system analyses for (Figure 1):

a. physical and logical structure identification and operation modes definition;
b. identification of the propagation phenomena/dynamics in the critical infrastructure;
c. identification of the interactions among several critical infrastructures.

In this thesis, four modeling approaches have been devised to perform these analyses resorting to the complex network theory method (Figure 1):

- topological unweighted network analysis to address issue a);
- weighted network analysis to address issue a);
- cascading failure dynamics analysis to address issue b);
- dependencies and interdependencies identification and modeling to address issue c).

Recent advances in complex systems theory indicate that many complex systems are hierarchies of networks of interacting components. In this view, the actual structure of the network of interconnections among the components is a critical feature of the system. Unweighted networks, i.e. networks that have a binary nature, where the edges between nodes are either present or not, can be subject to topological analysis. In a topological analysis, a CI is represented by a graph *G(N, K)*, in which its physical constituents (components) are mapped into *N* nodes (or vertices) connected by *K* unweighted (all equal) edges (or arcs), representing the links of physical connection among them. The focus of topological analysis is on the structural properties of the graphs on the global and local scales, e.g. as represented by, respectively, their characteristic path length, *L*, defined as the number of arcs in the shortest path between two nodes averaged over all pairs of nodes, and average clustering coefficient, *C*, a measure of the extent to which nodes tend to form small groups. Average global measures, such as *L*, give indications on the extent to which each node *i* in the system is connected with any other node *j*, while average local measures, like *C*, assess to what extent the first neighbors of each node *i* are connected among each other.
In spite of the usefulness of the topological analysis of the unweighted network of a CI and of the insights it provides, empirical results show that it cannot capture the rich and complex properties observed in a real infrastructure system, so that there is a need for extending the models beyond pure unweighted, structural topology.
Indeed, along with a complex topological structure, many real networks display a marked physical heterogeneity in the capacity and intensity of the connections. To describe the inhomogeneities of real physical systems, numerical weights can be assigned to each link of the representative network, measuring the 'strength' of the connection. By considering the 'reliability distances' among network nodes in terms of the probabilities of failure of the interconnecting links, global and local reliability efficiency indicators can be defined for use in the analysis of the robustness and vulnerability of network systems and thus for their optimal design, operation and management. Reliability weighted analysis has been applied:

- to evaluate the service reliability efficiency of the tramway network system of the city of Milano, Italy;
- to analyze the safety of a section of the road network of Piacenza Province in Italy;
- to assess the power transmission network properties and transmission performances of the Swiss 220 kV / 380 kV high voltage transmission system.

In real network systems, another important dimension to add to the vulnerability characterization refers to modeling the dynamics of flow of the physical quantities in the network. This entails considering the interplay between structural characteristics and dynamical aspects. These models provide indications on the elements critical for the propagation process and on the actions that can be performed in order to prevent or mitigate the undesired effects. Abstract modeling paradigms for analyzing the system response to cascading failures have been developed to capture the basic realistic features of CI networks within a weighted topological analysis framework.
Finally, dependencies and interdependencies among different CIs have to be modeled for assessing the influences and limitations which interacting infrastructures impose on the individual system operating conditions. Infrastructure interdependency stems from the functional and logical relations among individual components in different distributed systems. In order to characterize the extent to which a contingency affecting an infrastructure is going to weaken, and possibly disrupt, the safe operation of an interconnected system, it is necessary to model the relations established through the connections linking the multiple components of the involved infrastructures. The modeling of interdependencies among network systems and of their effects on failure propagation can be carried out within the simulation framework of failure cascade processes; the sensitivity of the coupling parameters defining the interdependency strength is of particular interest for the definition and prescription of cascade-safe operating margins in interdependent CIs.

THERMOPHORESIS IN COMPLEX FLUIDS

Daniele Vigolo

The work of my Ph.D. had the purpose to investigate nonequilibrium effects arising in "complex fluids" by means of optical methods. The research done has been experimental, eventually involving the development of an existing apparatus. The application field is the so called soft condensed matter physics, more specifically complex fluids (in particular nanometer-size latex particles, surfactant micelles or polymer suspensions) in the presence of thermal gradients.

When a colloidal suspension is placed in a temperature gradient, the dispersed particles display, on top of Brownian motion, a steady drift velocity. Then, depending on the system, particles can concentrate either at the cold (and in that case they are usually dubbed "thermophobic") or at the hot side (and they are conversely called "thermophilic"), i.e. the mass flow can be either along or opposite to the temperature gradient, leading to a steady state concentration gradient.

The stationary state is a nonequilibrium state, and this phenomenon is properly described into the frame of nonequilibrium thermodynamics. Mass diffusion coupled to a temperature gradient can be observed in both liquid and gaseous binary systems. In liquids, thermal diffusion was observed for the first time in electrolyte solutions by Ludwig, and then systematically studied by Soret. Thermal diffusion in liquid mixtures is indeed commonly known as Soret effect, while the same phenomenon in colloidal dispersions is usually referred to as thermophoresis. Investigation of the Soret effect is extremely important for various research areas and different technological applications, as:

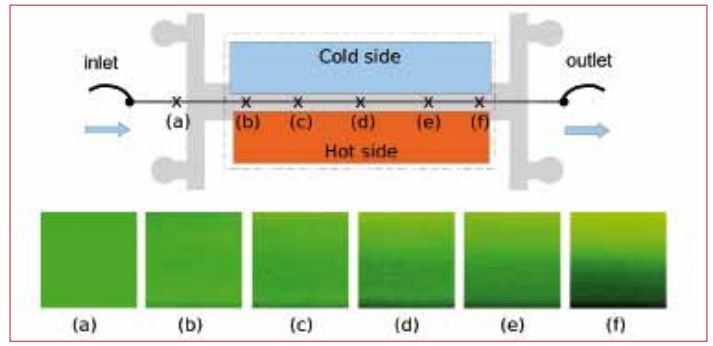
- analysis of fluctuations and convective instabilities in multicomponent systems driven by concentration gradients;
- crude oil industry. In fact concentration distribution and geothermal gradients may induce local variations in composition due to thermodiffusion effects;
- segregation processes ranging from component differentiation in solidifying metallic alloys to isotope separation;
- optical fibers manufacturing, where thermophoresis is the dominant mechanism of silica particle deposition onto a rotating cylindrical target;
- biotechnological applications such as in the protein crystal growth or in the concentration and replication of DNA.

Despite its relevant applications and although known since a long time, the Soret effect still lacks a general microscopic picture, especially in the less studied case of aqueous solutions. Colloidal and nanoparticle systems, however, lend themselves to a simpler, semi-microscopical approach. Colloids are indeed much greater than solvent molecules which can be regarded as a continuum medium. In this case, the analysis must be focused on what happens at the particle-solvent interface when a temperature gradient is applied. Suggestions have appeared in the literature, for the interpretation of thermophoretic motion of particles suspended in a liquid as an interfacial tension gradient driven phenomenon.

In the last few years, noticeable experimental efforts have been made to investigate thermophoretic effects in a wide class of complex fluids, ranging from model colloidal suspensions, to polymers, surfactant solutions, and biological fluids, while extensive theoretical investigations have been devoted to unravel the basic mechanisms underlying thermophoresis. The most distinctive feature of these results is the strong dependence of thermophoresis on the nature of the investigated system and on solution parameters such as temperature, ionic strength, or pH, rendering in principle thermophoresis much more "selective" than other particle–driving mechanisms. Exploiting thermophoresis to manipulate colloids or macromolecules is an alluring perspective. In fact, careful control by thermal gradients of colloidal crystal growth has already been proved to be fully feasible.

Starting from this "state of the art", my Ph.D. work lead to several relevant results. Namely I studied how particles size, isotopic substitution or thermal expansivity change in the solvent and the kind of electrolytes dispersed in the solution can influence the magnitude of thermophoresis and the direction of motion of the particles.
The most relevant results can be summarize as follow:

- I found a linear behavior of the Soret effect with the particle size by studying aqueous dispersion of latex spheres of different sizes carefully standardizing the particle surface in order to keep constant the particle-solvent interaction;
- deeply analyzing the influence on the kind of electrolyte on charged surfactant micelles, I found that it can be possible, by simply changing the ratio of two different kinds of electrolyte, to continuously adjust intensity and direction of the charged particles drift keeping constant the total amount of dispersed charge. A fully concentration dependence in the presence of different electrolytes is also given by studying the osmotic compressibility of the system.



1. (a{f) Fluorescence images showing the accumulation of particles to the cold side. The experiment uses 477nm diameter PS particles in the presence of 100mM NaCl with a flow rate of 0.01 μl=min ≃ 90 m=s

Then, an application of thermophoresis as a microfluidic separator was tested. The so called microfluidic lab-on-chips are usually designed to mimic on a much smaller scale operations performed in a standard laboratory, with the significant bonus of greatly reducing the amount of sample and the time needed to perform a specific task. The transversal size of the channel that is only few tenth of microns, gives the possibility to exploit the separation capability of thermophoresis as the time scale depends on mass diffusion. Moreover, thermophoresis allows to discriminate particles based on their surface interactions with the solvent, which let thermophoresis be not only an alternative to standard way to manipulate particles in microfluidics geometry but also a method to actually separate mixed species otherwise hard to discriminate. During a period working in the laboratories of Prof. Howard A. Stone in Harvard University, USA, I designed and successfully tested this kind of device. As shown in the attached figure, by applying a difference in temperature across a microchannel, it is possible to accumulate particles in one side (depending on the system and, for instance, on the presence of specific electrolytes that would be the hot or the cold side).