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.

The specific thesis discussed in this Yearbook are related to the Phd work of:

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COMPUTATIONAL METHODS FOR THE PERFORMANCE ASSESSMENT OF RADIOACTIVE WASTE REPOSITORIES

Diana–Maria Avram

The appropriate disposal of radioactive wastes is a technical challenge due to the long periods of time needed for the radioactivity to decrease below acceptable safety levels established by the competent regulatory agencies. The disposal requires isolation from the environment provided by a system of engineered and natural barriers, whose objective is to prevent and retard the radionuclides release and migration to the groundwater and eventually to the biosphere. The quantitative analysis of the processes of radionuclide migration across the barriers to the main intake paths plays a fundamental role in the safety performance assessment of the overall system.

The performance assessment (PA) of the radioactive waste repositories involves the systematic analysis of the containment structure in order to investigate the events and processes that influence its behavior. Eventually, it is required the estimation of the expected dose to some defined critical individual, with the associated aleatory and epistemic uncertainty. Therefore, predictive mathematical/computer models are relied upon in the PA to adequately represent the evolution of physical processes that may release, transport and ultimately lead to radiological exposure. Nevertheless, the complexity of the phenomena and geometries involved implies running elaborate simulations and large computer codes, with significant time and memory expenditures, when performing the analysis necessary to assess the reliability of the model outcomes.

For this reason, the work presented in this Ph.D. thesis, has focused on the investigation of strategies for the development of computational procedures of system analysis and for acceleration of model computation for the PA of radioactive waste repositories. The strategies employ the use of advanced simulation techniques (e.g., Monte Carlo) to address the problem of incorporating realistic features in the modeling of the barriers, Subset Simulation technique for increasing the efficiency of parameters random sampling and empirical meta–models for large codes approximation. The research activity lies within the PA methodology and is organized as follows:

- *Model simplification*: simplified reliability–based models for evaluating the long-term functionality of the repository barriers system in terms of system failure time distribution and of doses to the critical individual;
- *Model acceleration*: methods for fast computation:
  - Subset Simulation technique for improving the efficiency of random sampling for estimating small repository containment failure probability;
  - Gaussian process–based meta–models for replacing the large computer codes by reduced models (response surfaces) with acceptable calculation times.

Model simplification for the PSA of radioactive waste repositories

The failure of the engineered barriers is affected by phenomena of water infiltration and degradation, but also of cracking due to settling of the structure under gravity forces or temperature-induced volume changes. On account of the complexity of failure mechanism and occurring processes an analytic treatment of the problem would be impractical, rendering the numerical schemes mandatory. In this regard, a Monte Carlo (MC) simulation–based reliability model of the multi-barrier system has been developed for the preliminary evaluation of the repository long-term functionality within a Probabilistic Safety Assessment (PSA) framework. The MC simulation-based approach addresses the problem of estimating the repository barriers failure time distribution and the associated doses to the critical individual. The aim is that of providing a lean modeling framework for performing initial evaluations of the barriers performance within a simplified scheme of calculations which allows a quick and relatively light analysis, while offering the flexibility for maintaining the necessary realism in the description of the failure and transport processes. Moreover, the strategy confers certain modularity to the MC-based probabilistic model, which, for demonstration purposes, has been combined with the numerical solution of flow and transport processes in the aquifer.

Model acceleration: Subset Simulation

The uncertainties in the parameters governing the probabilistic modeling of the release processes are taken into account and described in terms of probability density functions (pdfs); their propagation to the reliability model output allows estimating the probability that the dose exceeds the regularity limits. The Subset Simulation, specifically developed to tackle the multidimensional problems of structural reliability, is adopted for improving the efficiency of the random sampling of the parameters and for estimating the small containment failure probability. In practice, the protective barriers are designed to be very reliable so that their failure is a rare event; in a standard scheme based on sampling the uncertain parameters distributions and computing the corresponding doses would require many code runs and, thus, large computational times for obtaining a statistically robust estimate. To this aim, an original analogy to the problems of structural reliability is proposed with regards to the quantitative analysis of the failures of the multi-barrier system of a radioactive waste repository, where the failures are specified in terms of one or more safety variables crossing the safety thresholds. Moreover, the Subset Simulation peculiar set-partitioning scheme is exploited for performing the analysis of the sensitivity of the failure probability estimate to the uncertain model parameters.

Model acceleration: Gaussian process–based meta–models

The second approach to model acceleration consists of an original combination of Gaussian Process-based (GP) meta-models with a space reduction technique, Principal Component Analysis, for predicting the time-dependent radionuclide concentration in groundwater, following a release from a radioactive waste repository. Another contribution of the work consists of an analysis of the possibility of having a priori information on the meta-models prediction capability, i.e., either before constructing it or after. In this respect, a "backward" analysis has been performed for gaining some insight on how the positioning of the input training samples with respect to the test samples influences the meta-model prediction capabilities and the presence of the outliers, e.g., large uncertainty present in the predicted outcome. This is particularly helpful when dealing with complex, multi-dimensional prediction problems, characterized by many input variables and the meta-model design case requires a lot of calibration efforts.

QUANTITATIVE TECHNIQUES FOR THE VULNERABILITY ANALYSIS OF CRITICAL NETWORK SYSTEMS AND INFRASTRUCTURES

Lucia Golea

Problem statement

The subject of this Ph.D. thesis is the analysis of critical network systems and infrastructures with respect to their vulnerability to random failures and targeted attacks. 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, Italy, founded by the Institute for an Industrial Safety Culture (ICSI) of Toulouse, France.

The motivation is that critical infrastructures (CI) provide the continuous flow of essential goods (e.g. energy, water, data) and services (e.g. banking, health care, transportation) which the welfare and security of our nations rely on. The focus of the research work was on the modeling of CI as complex systems from the standpoint of network theory. The basic concept of network theory is to build an abstract model of real-world networks and describe the form and, in various degrees, the function of the network by different measures.

Research performed

Figure 1 shows the researches carried out during the Ph.D.

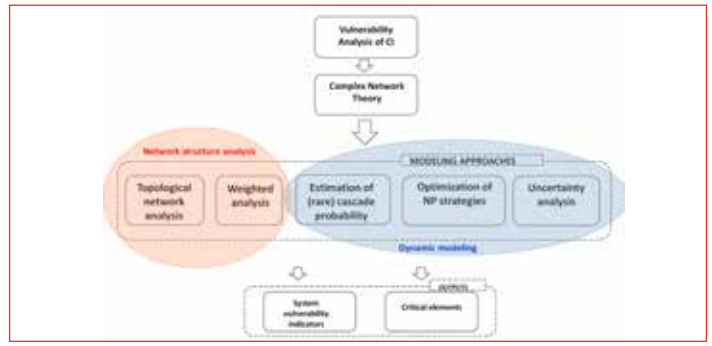
In the *topological network analysis* performed, the CI is represented by a graph G(*N*, *K*), in which its components are mapped into *N* nodes connected by *K* unweighted edges, representing the links of connection among components. In order to quantify the structural importance of the network components, several centrality measures have been introduced (e.g. the group degree, closeness and betweenness centrality) and the most important groups of elements of different sizes in the network have been identified. The identification of the most central groups is a combinatorial problem which has been tackled by Genetic Algorithms (GA). The multi-objective GA framework has been tested on the electrical transmission network test system IEEE 14 BUS and it was observed that critical groups of components may include components that are not critical when considered individually. Therefore, the criticality of these components may be underestimated if the importance ranking is performed only with respect to individual components.

While the topological approaches for identifying critical components are capable of highlighting structural vulnerabilities, they are limited from the point of view of the functional analysis of the CI. The Italian high-voltage electrical transmission network has been taken as case study for the analysis of the importance of groups of edges from the viewpoint of the network structure and flow. The results of the pure topological analysis, were compared to the results of the vulnerability analysis complemented by functional information on the network. It has been shown that the topological approach requires minimum information of the network and leads to the identification of a number of critical edges that have also "functional" relevance.

In spite of the usefulness and of the insights provided by the topological analysis of the unweighted network, empirical results show that it can capture only partially 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.

In this view, the formalism of *weighed networks* has been exploited to provide different graph-theoretical representations and analyses of a power transmission system. Four different perspectives of analysis were considered within the formalism of weighed networks, adding to the purely topological analysis of the system the reliability and electrical characteristics of its components. The electrical transmission network IEEE RTS 96 has been taken as reference for the analysis. Based on the comparative evaluation of the four perspectives with respect to other approaches for vulnerability assessment, we proposed a framework that incorporates the four perspectives presented in a preliminary screening analysis of network vulnerability. By performing such an analysis, a better comprehension of the system is achieved, and the different criticalities within the network components are highlighted.

By nature, topological, weighted or unweighted, analyses focus on the static properties of a network. A further important dimension to add to the vulnerability characterization of CI refers to modeling the dynamics of flow of the physical quantities. From the abstract modeling of a cascading failure propagation process, it has been possible to accurately *estimate*, by Monte Carlo Simulation (MCS), *the probability of cascading failure under given load conditions*. To overcome the computational problems of standard MCS, the Subset Simulation (SS) method has been implemented. Such method circumvents the computational burden associated to the estimation of a small failure probability by computing it as a product of larger conditional probabilities of more probable intermediate events.



1. Pictorial view of the critical infrastructure vulnerability analysis performed in the Ph.D. research work carried out at LASAR.

The problem of *optimization of protection strategies in critical infrastructures* within a complex network systems perspective was also addressed. Three different protection strategies were proposed that minimize the consequences of cascading failures on the entire system, on predetermined areas or on both scales of protective intervention in a multi-objective optimization framework. We optimized the three protection strategies by devising a modified binary differential evolution scheme that overcomes the combinatorial complexity of this optimization problem. We exemplified our methodology with reference to the topology of an electricity infrastructure, i.e. the 380 kV Italian power transmission network.

In the final step of the CI analysis, the *characterization of uncertainties related to electric transmission networks* has been undertaken. In order to quantify the impact that the propagation of the identified uncertainties has on the reliability of the electric infrastructure we developed a stochastic model that simulates the operations of the electric network. The event-based model was embedded in the MCS framework and has shown the ability to represent daily hourly changes in power requests at customer side of the system, room temperature and wind speed. We noticed that increasing variability in the operating conditions lead to an increase in the generated power that may not reach the customers.

Conclusions

The results of this thesis work support the belief that the methods of complex network theory can provide information useful for the vulnerability assessment of CIs, within a screening analysis of their behavior. The screening analysis can be supported by structural information provided by system owners and operators, including the general understanding of main functionalities, interfaces and interdependencies. The evaluation of the statistical indicators derived from the methods of complex network theory can highlight preliminary vulnerabilities, e.g. structural or reliability bottlenecks, which must be the focus of a successive detailed system analysis.

MODELLING OF FISSION GAS SWELLING AND RELEASE IN OXIDE NUCLEAR FUEL AND APPLICATION TO THE TRANSURANUS CODE

Giovanni Pastore

The context of the present Ph.D. thesis is the domain of research oriented toward the computational thermo-mechanical analysis of the nuclear fuel rods (fuel rod modelling). The emphasis is on the analysis of pellet-in-cladding type uranium dioxide (UO_2) fuel for light water reactors (LWRs), which constitute the majority of nuclear power reactors operated presently. The work was carried out in the frame of a collaboration between the Politecnico di Milano and the JRC/ITU (Joint Research Centre / Institute for Transuranium Elements).

LWRs employ fuel in the form of rods comprised of ceramic fuel pellets (generally UO_2) piled-up in a zirconium-alloy cladding tube. Besides providing the heat generation and transfer to the coolant, the fuel rod is the first and the second barrier (i.e., the fuel pellets and the surrounding cladding tube, respectively) to the release of the radioactive fission products to the environment, and therefore plays a primary safety role.

The aim of fuel rod modelling is to predict the thermo-mechanical behaviour and lifetime of the nuclear fuel rods. The strong interrelationship between the several, intricate phenomena taking place in the fuel rod during irradiation in the reactor, as well as the non-linearity of many processes involved, calls for the development of computer codes analysing the general fuel rod behaviour. The fuel rod analysis codes are presently used by industries, research centres, universities and safety authorities, in support of fuel characterization, design and licensing. In this framework, the TRANSURANUS fuel rod analysis code, developed at the JRC/ITU, is the most widely adopted tool in the European Union. The progress of fuel rod modelling is supported by many International Projects. In particular, the present thesis was carried out within the FUMEX-III (FUel Modelling at EXtended burn-up) co-ordinated research project of the IAEA (International Atomic Energy Agency).

Among the various issues involved in fuel rod modelling, the behaviour of the fission gases xenon and krypton represents a challenging task in view of the complexity of the relevant physical mechanisms and the strong implications on the thermo-mechanical behaviour of the fuel rods.

On the one hand, the fission gases generated in the fuel tend to precipitate into bubbles resulting in fuel swelling (volumetric and permanent deformation), which may give rise to enhanced pellet-cladding mechanical interaction (PCMI).

On the other hand, the inter-connection of the gas bubbles developing at the fuel grain boundaries leads to fission gas release (FGR) to the free volume of the fuel rod, which causes pressure build-up and thermal conductivity degradation of the rod filling gas. The inherently coupled kinetics of fission gas swelling and release calls for the development of physics-based, integrated models of these phenomena to be employed in the fuel rod analysis codes. As of today, however, empirical approaches are widely adopted, which are inexpensive to use but unfit for providing insight into the underlying mechanisms, and cannot be applied beyond their range of calibration. A further open issue concerns the dependence of both fission gas swelling and release on the hydrostatic stress in the fuel, which is often neglected or treated in a simplified way in view of the involved complexity of the numerical treatment.

The present thesis represents a contribution to the modelling of fission gas swelling and release in the fuel rod analysis codes. The work comprises (i) a development aspect, which entails the construction of a physics-based and integrated model of fission gas swelling and release in UO_2 fuel during irradiation, properly taking into account the intrinsic coupling as well as the dependence of both phenomena on the hydrostatic stress, and (ii) an application aspect, including the implementation in the TRANSURANUS code, the employment in fuel rod analyses and the verification of the model.

Through an engineering modelling approach, which practically combines a physics-based treatment and the simplicity that is a prerequisite for the effective application to the fuel rod analysis codes, a new model with the above characteristics was developed. The model describes the relevant processes of gas diffusion and precipitation, bubble growth and inter-connection, providing a consistent, integrated treatment of the fission gas swelling and release.

As a first step of verification, the model was coded as stand-alone version and applied to the analysis of either power ramped or power cycled UO_2 fuel specimens. The model was proven to consistently reproduce the main peculiarities of the fission gas behaviour, in accordance with the observations reported in the literature. A first quantitative assessment was carried out of the predictive capability of the model against a dataset of swelling measurements from the OECD/NEA (Organisation for Economic Co-operation and Development / Nuclear Energy Agency) International Fuel Performance Experiments database, pointing out a reasonable predictive accuracy, without fitting of the model parameters.

The applicability of the new model to fuel rod modelling (hence, to the nuclear fuel design and licensing) was demonstrated by successful implementation in the TRANSURANUS fuel rod analysis code. During the implementation, consistent matching was provided between the non-linear, stress-dependent model calculations and the thermo-mechanical fuel rod analysis. Numerical stability and reasonable computational times were obtained.

Adopting the new model, the TRANSURANUS code was employed for an extensive set of simulations of LWR-UO_2 fuel rods irradiation experiments involving power ramps. The coupling between the fission gas swelling and release, and the dependence of both phenomena on the hydrostatic stress, were confirmed to be reproduced consistently with the experimental observations. Moreover, the assessment of the results against experimental data of FGR pointed out a satisfactory agreement, without applying any tuning to the model parameters.

The implementation of the new model represents a significant progress in the development of the TRANSURANUS code. The innovative aspects are mainly related to (i) the advantages of a physics-based and integrated treatment in terms of flexibility of application and understanding of the underlying mechanisms, compared to the previously adopted empirical approaches, (ii) the observed improvement of the predictive accuracy in terms of FGR, and (iii) the consistent evaluation of the dependence of both fission gas swelling and release on the hydrostatic stress. The latter aspect is of high importance in view of the current tendency to extend the flexibility of use (load-following) and the discharge burn-up of the nuclear fuel, which can involve the occurrence of strong PCMI and the consequent development of high hydrostatic stress in the fuel due to cladding restraint.

The current results are promising in view of future applications of the model, implemented in the TRANSURANUS code, in both research and industrial frameworks. Also, the successful implementation in the TRANSURANUS code indicated that the model may be of interest for application to other fuel rod analysis codes.

To summarize, the general features of the model developed in the present thesis, in terms of physical foundation and computational efficiency, constitute a framework that allows the application to fuel rod modelling of the physics-based, integrated and stress-dependent treatment of the fission gas swelling and release. The underlying approach is generally applicable and can be reproduced in order to develop increasingly complex and advanced models with the above fundamental capabilities to be implemented in the fuel rod analysis codes. Therefore, in addition to some specific modelling aspects, the basic engineering approach constitutes, in essence, the most significant and innovative contribution of the work.

RARE EVENTS IN MANY-BODY SYSTEMS: REACTIVE PATHS AND REACTION CONSTANTS FOR STRUCTURAL TRANSITIONS

Massimiliano Picciani

In several domains, like material sciences, chemistry and even biology, the evolution of multi-particle systems is often governed by thermally activated processes having a dramatic effect on the structure. These physical events consist of passages between different stable configurations of the system, separated by energetic or entropic barriers. As they usually occur with a very low probability, they are indicated as rare events; their frequency, described by the reaction rates, fully determines the global kinetics of the system via its master equations. Examples of physical phenomena controlled by such rare events are protein folding in biology, defect diffusion and crystal nucleation in condensed matter physics and cluster rearrangement in chemistry.
Rare events are characterized by the fact that the typical time needed for them to start is very large, while their duration is rather short, e.g. of the order of the picoseconds in dense molecular systems. This separation of time-scale is the very definition of metastability; its origin may be energetic or, more likely in high dimensional systems, at least partly entropic, when is related to pathways hard to find. Both features (energetic and entropic) are investigated once one resorts to a free energy description of the activation barrier, able to take into account temperature effects. There are two main issues in the study of rare events: the determination of reactive paths and the computation of reaction rates.
First, reactive paths linking the initial state to the final one have to be found. This problem is intimately related to the exploration of the free energy landscape of a multi- particle system. The determination of reactive paths is connected to the topology of the energy landscape underlying the system dynamics, and requires the localization of transition regions separating stable states. These regions have often a complex conformation, being constituted not only by simple barriers, but by a sequence of saddle point and intermediate metastable basins. This implies, in turn, the problem of the construction in many body systems of reaction coordinates able to accurately discriminate different stable and unstable configurations. Indeed, handling and visualizing systems with a large number of degrees of freedom requires the elaboration of collective coordinates, i.e. a few variable given by functions of the total number of configurational degrees of freedom. Very well known examples of collective variables are the bond-orientational order parameters, that are a function of the distances between all particles composing the system. However, the degree of coarse-graining (i.e. the reduction of the number of configurational variables used to describe the system) related to these reaction coordinates needs to be not too strong, in order to avoid a loss of information on the system structure, and subsequently a wrong representation of the energy landscape: in some cases, for example in the study of crystalline symmetries, order parameters take values that do not correspond one-to-one to the different states of the system. This problem worsen when a precise description of the position of transition states in phase space is needed in order to compute quantities like reaction rate (see below), as using inadequate reaction coordinates can induce poor numerical estimations. The exploration of energy landscapes of complex systems is, for these reasons, a very broad research field, and several exploration techniques have been proposed in the past. Moreover, the relation between reactive paths, diverging trajectories and instability in dynamical systems is deeply exploited in this work for the determination of the first ones. The theoretical basis of this relationship is given by the Lyapunov instability theory, that pro- vides observables, called Lyapunov exponents, enabling to quantify the degree of chaoticity on a dynamic system. Chaoticity can be indeed related to the potential energy surface conformation via the spectra of the hessian matrix and transition regions are indeed regions of unstable dynamics. Hence, the determination of diverging trajectories helps in finding barriers separating stable states.
The second issue in rare events studies concerns the determination of the frequency at which these events happen. This frequency is usually indicated as reaction rate, and is indeed a way to quantify "how rare" these events are.
A large variety of approaches have been proposed in the past in order to obtain a theoretical description of reaction rates, the most important being the transition state theory elaborated by Eyring, Kramers and others, as well as the "mean first passage time" approach.
The fundamental hypothesis for reaction rate theories is again the presence of a well defined separation of time scales: the time that one has to wait in order to see a rare event happening is much larger than the time needed to the system to relax in a given state. The computation of reaction rates is usually related to intermediate time scales between these two times.
In this PhD thesis, both problems of characterizing reactive paths and evaluating associated reaction constants have been addressed. The first study, focused on the characterization of reactive paths, is presented in details in Chapter 2, and consists of a method called transition current sampling (TCS), derived from a reformulation of the Lyapunov-weighted dynamics of Tailleur and Kurchan.
This method is based on the numerical simulation of the probability currents flowing between stable and metastable states, and derives from the SuperSymmetric Langevin dynamics mentioned above.
The theory guarantees that by selecting trajectories having larger Lyapunov exponents, the bias is just what is needed so that the population describes the evolution of the transition current, rather than the evolution of configurations, as it would in an unbiased case. The advantage is that the convergence of the current distribution is much faster than the typical passage time. The method and its validation have been published as "Simulating structural transitions in transition current sampling: the example of LJ 38", in Journal of Chemical Physics.
The second study is motivated by the necessity of computing reaction constants. This was difficult to achieve within the transition current sampling approach, as TCS is based on the numerical simulation of probability currents, rather then probability distribution. Therefore we elaborated a new approach connected to TCS, that consists in exploiting the advantageous features of a transition path sampling in terms of the computation of reaction constant, but introducing at the same time a bias based again on Lyapunov exponents. This bias can subsequently be removed in the evaluation of reaction rates resorting to an adequate unbiasing statistical tool, the MBAR method. This second work, named local Lyapunov biased transition path sampling (LyTPS) is presented in Chapter 3, and has been submitted to the Journal of Chemical Physics as "Calculation of reaction constants using transition path sampling with a local Lyapunov bias".
This last method is finally applied to the study of thermally activated events occur- ring in materials of nuclear interest. In particular, the focus was set on post-irradiation point defect migration in crystals, namely vacancies and divacancies, where the migration mechanism and the involved time scales allow a description based on rare events theory. We employed the method developed in Chapter 3 to compute migration rates and give an estimate of migration entropies. The results obtained are reported in Chapter 4, and have been presented in a proceedings for the conference MRS fall meeting 2011. Migration rates computed are subsequently employed in order to simulate resistivity recovery, and numerical results are furthermore compared with experiments.