

An Industrial Viewpoint on Uncertainty Quantification in Simulation: Stakes, Methods, Tools, Examples

Alberto Pasanisi¹ and Anne Dutfoy²

¹ EDF R&D. Industrial Risk Management Dept.
6 quai Watier, 78401 Chatou, France

² EDF R&D. Industrial Risk Management Dept.
1 avenue du Général de Gaulle, 92141 Clamart, France
{alberto.pasanisi, anne.dutfoy}@edf.fr

Abstract. Simulation is nowadays a major tool in R&D and engineering studies. In industrial practice, in both design and operating stages, the behavior of a complex system is described and forecast by a computer model, which is, most of time, deterministic. Yet, engineers coping with quantitative predictions using deterministic models deal actually with several sources of uncertainties affecting the inputs (and occasionally the model itself) which are transferred to the outputs. Therefore, uncertainty quantification in simulation has garnered increased importance in recent years. In this paper we present an industrial viewpoint of this practice. After a reminder of the main stakes related to uncertainty quantification and probabilistic computing, we will focus on the specific methodology and software tools which have been developed for treating this problem at EDF R&D. We conclude with examples illustrating applied studies recently performed by EDF R&D engineers arising from different physical domains.

Keywords: Simulation, Computer Experiments, Risk, Uncertainty, Reliability, Sensitivity Analysis.

1 Introduction

Computer simulation is undoubtedly a fundamental issue in modern engineering. Whatever the purpose of the study, computer models help analysts to forecast the behavior of the system under investigation in conditions which cannot be reproduced in physical experiments such as accident scenarios, or when physical experiments are theoretically possible but at a very high cost.

The need for simulating and forecasting gained dramatic momentum in recent decades due to the growth of computers' power and vice versa. Since the very first large scale numerical experiments carried out in the 40's, the development of computers (and computer science) has gone pairwise with the desire to simulate more and more deeply, more and more precisely, physical, industrial, biological, economic systems. A profound change in science and engineering has resulted

in which the role of the computer has been compared to the one of the steam engine in the first industrial revolution [1]. Together with formulating theories and performing physical experiments, computer simulation has been labeled a “third way to Science” [2] allowing researchers to explore problems which were unaffordable in a not so distant past. In turn this has raised epistemic issues.

Some scholars identify a shift from a scientific culture of calculation, linear, logical, aiming to simplifying and unpacking results, to a culture of simulation, empirical, opaque, aiming at providing high-dimension results, under nice forms of graphs, or even movies, (see [3] for an interesting discussion). A quite negative perspective of computer models, seen as opaque boxes one can play with to obtain whatever desired result, has also emerged which directly attacks the credibility of computational models as tools for guiding decisions [4].

Our viewpoint is pragmatic. We believe that computer simulation can serve as a major tool in daily engineers’ work and is furthermore capable to assist in understanding, forecasting, and guiding decision making. The possibility to simulate more and more complex phenomena, taking into account the effect of more and more input parameters is better viewed as an opportunity as opposed to a threat. However, at the same time, we are aware that quantitative uncertainty assessment of results is a fundamental issue for assuring the credibility of computer model based studies and remains a challenge as well.

Besides technical and theoretical difficulties, in industrial practice a key difficulty is to bridge the cultural gap between a traditional engineering deterministic viewpoint and the probabilistic and statistical approach which considers the result of a model as an *uncertain* variable.

Even if the fundamentals of these topics are rooted in probabilistic and statistic literature from decades back, in recent years there has been a significant increase in interest on the part of industries and academia in uncertainty quantification (UQ) applied to computer models. A casual survey of recent papers reveals the variety of disciplinary fields involved: e.g. nuclear waste disposal [5], [6] (which was also one of the first contexts in which UQ on large computer models was applied), water quality modeling [7], avalanche forecasting [8], welding simulation [9], buildings performance simulation [10], galaxies formation [11], climate modeling [13], fires simulation [14] to name a few.

The remainder of the paper is organized as follows. Section 2 presents the common framework for uncertainty assessment as it is currently used in the industrial practice by EDF (Électricité de France) and other major stakeholder companies and industrial research institutions, for example: European Aeronautic Defence and Space Company (EADS), French Atomic Energy and Alternative Energies Commission (CEA), and Dassault Aviation. Uncertainty analysis requires a multi-disciplinary approach, and this framework is an useful tool to establish dialog between experts in the disciplinary field of the model application and those with a more probabilistic or statistical background. It also allows to put into evidence, at the very early stage of the study, what is the really relevant expected outcome and, consequently, to choose the most proper and effective mathematical tools to obtain it.

Section 3 presents *Open TURNS*, an open source software package, jointly developed by the three companies EDF, EADS and Phiméca, which implements the methodology described in Section 2. Together with proper and recent mathematical algorithms, an interesting feature of Open TURNS is that it can be linked in an effective and rather easy way to any external computer code, which is simply seen as a deterministic function of a random input. By a mathematical viewpoint, that corresponds to linking a deterministic model to a probabilistic model of its inputs.

Section 4 shows some practical examples of applied studies carried on at EDF. These studies concern different problems and involve a great variety of physical problems. The wide range covered by those examples, due to the diversity of EDF's business areas, illustrates the motivation for both a general approach to the problem, as well as the need for specific and powerful mathematical and software tools.

Section 5 very briefly sketches some conclusions and perspectives.

2 The Common Framework for Uncertainty Management

2.1 An Iterative Methodology in Four Steps

In the last decade, thanks to the numerous multi-disciplinary challenges it has to cope with, EDF established a global methodology for uncertainty treatment for models and simulations. This framework has subsequently been accepted and improved by other industrial and research institutions.

The EDF focus is on so-called parametric uncertainties, i.e. uncertainties characterizing dispersion of input parameters of a model, where a model could be a complex numerical code which requires an approximated resolution or an analytical expression. Our analysis does not explicitly address uncertainties attached to the computer model itself, arising from simplifying assumptions for the model of the physical phenomenon under investigation, nor numerical uncertainties due to its practical implementation as a computer code. The methodology is based on the probabilistic paradigm, i.e. uncertainties are represented by associated probability distribution functions (pdf). Even if some perspective works are carried at EDF R&D on extra-probabilistic approaches [15], they are currently considered not yet sufficiently mature for engineering application.

The common framework of uncertainty management is a four step process the genericity of which facilitates application across a broad variety of disciplinary fields: (i) *Step A "Uncertainty Specification"* defines the structure of the UQ study by selecting the random parameters, the outcomes of interest and the features of the output's pdf which are relevant for the analysis; (ii) *Step B "Uncertainty Quantification"* defines the probabilistic modeling of the random parameters; (iii) *Step C : Uncertainty Propagation* evaluates the criteria defined on Step A; (iv) *Step C' "Uncertainty Importance Ranking"* determines which uncertainty sources have the greatest impact on the outcome (sensitivity analysis).

In practice, the process is often iterative: a too large uncertainty tainting the final outcome and/or the ranking step could motivate corrective feedback R&D actions for reducing uncertainties where possible, e.g. setting up new experiments to improve the probabilistic modeling of model's inputs.

The following sections review the principal methods used in each step of the framework.

2.2 Step A - The Uncertainty Problem Specification

This step first involves selection of the input parameters to be represented as random variables. The remaining parameters are considered as fixed either because they are supposed to be known with a negligible uncertainty or (as it is typical in safety studies) because they are given values, generally conservative, which are characteristic of a given accident scenario. In the following we will denote by X the vector of the random input parameters, and $Z = G(X)$ the random outcome of interest of the deterministic model $G(\cdot)$.

Step A requires also to select the relevant features of the outputs' pdf, depending on the stakes which motivated the study (the so-called *quantities of interest*). In most cases they formalize, in a simplified yet explicitly normative manner, some decision criteria. For instance, during the design stage of a system, the analyst is often asked to provide the mean and the standard deviation (or the range) of a given performance indicator of the system—e.g., fuel consumption—in order to check its general conception. Whereas in operating stages, one must often verify that the system satisfies (or not) regulatory requirements for licensing or certification. Therefore, depending on the context of the study, the decision criteria may be: (i) a *min/max* criterion, i.e. the range of the outcomes given the variability of the inputs; (ii) a *central dispersion* criterion, i.e. central tendency and dispersion measures; (iii) a *threshold exceedance* criteria, i.e. the probability for a state variable of the system to be greater than a threshold safety value.

A rudimentary analysis of the computer code is also necessary: does it require a high CPU time for a single run, does it provide a precise evaluation of its gradient with respect to the probabilistic input parameters are typical questions.

Depending on these considerations, the uncertainty quantification methodology proceeds through different algorithms.

2.3 Step B - The Input's Uncertainty Quantification

The methods used for the probabilistic modeling of the inputs depend on the nature and the amount of available information.

In case of scarce information, the analyst first needs to interview experts. The literature proposes numerous protocols (e.g. [16]) that can assist in obtaining unbiased and relevant information which may then be translated into a pdf. In addition, a commonly used approach consists in applying the Maximum Entropy Principle, that leads to the pdf maximizing the lack of information (modeled by the Shannon entropy [17]), given the available expertise on the variable to be modeled. Whatever the chosen model, it is critical to validate it. One means

for this consists of establishing a dialog with the expert to clearly identify key features for comparison with the established pdf—e.g. mean and quantiles, or alternative shape and scale parameters.

When data sets are available, the analyst can use the traditional statistical inference tools following a parametric or non parametric approach. The kernel smoothing technique is useful to model distributions which do not present usual shapes, for example, multimodal distributions. Then, the model is validated by a numerical fitting test, adapted to the objective of the analysis: for example the Kolmogorov test is used in the central zone or Anderson-Darling if one is more interested in tail fitting.

The EDF framework requires that the random input parameters X_1, \dots, X_m be represented as a random vector X with a multivariate pdf, the dependence structure of which must be explicit. A common way is to define the multivariate pdf $p(X)$ by its univariate marginal distributions $p_1(X_1), \dots, p_m(X_m)$ and its copula \mathcal{C} , the later encoding the dependence structure [18]. In practice, inference on copula parameters can present problems and, as shown in [19], Kendall's τ or Spearman's ρ coefficients are not sufficient to fully determine the structure. Mismodeling the dependence structure is potentially dangerous as it can lead to an error of several orders of magnitude in the estimate of a threshold exceedance probability [20]. Our recommendation is that the copula inference be performed using the same techniques (e.g. Maximum Likelihood Estimation) as those for the univariate marginals.

2.4 Step C - The Uncertainty Propagation

Once quantified, uncertainties are propagated to the model outcomes. The propagation algorithms depend on the decision criteria and on the model characteristics specified in Step A.

In case of a *min/max* analysis, the range of the outcome is determined either as a result of an optimization algorithm or by sampling techniques. The input sample may come from a deterministic scheme—e.g., factorial, axial or composite grid—or randomly generated from the distribution accorded to the input vector. The choice of the method is informed by the CPU time required for model execution, $G(\cdot)$.

In case of a *central dispersion* analysis, the mean value and the variance of the outcome can be evaluated using Monte Carlo sampling, which also provides confidence intervals of the estimated values. If a high CPU time forbids such a sampling method, it is possible to evaluate the mean of the outcomes using a Taylor variance decomposition method that requires the additional evaluation of the partial derivatives of the model $G(\cdot)$. No confidence interval is estimated to quantify the quality of the Taylor approximation.

Finally, in case of a *threshold exceedance* criteria $\mathbb{P}[G(x) \geq z^*]$, the most widespread techniques are the simulation-based, such as Monte Carlo method and its variants that reduce the variance of the probability estimator: LHS, importance sampling, directional sampling, . . . All of the simulation techniques provide confidence intervals. More sophisticated sampling methods exist to evaluate

rare events (e.g. particle sampling [21]). In case of high CPU runtime, alternatives (FORM and SORM methods) exist to estimate the exceedance probabilities, based on an isoprobabilistic transformations such as the Generalized Nataf transformation [20], [22] in case of elliptical copula of the input random vector, and the Rosenblatt one [23], [24] in the other cases. These transformations are designed to map the input random vector into a standard space of spherical distributions. In that space, the integral defining the exceedance probability:

$$\int_{\mathcal{D}_f} p(x)dx, \text{ where: } \mathcal{D}_f := \{x; G(x) \geq z^*\}$$

is approximated using geometrical considerations [25,26,27]. These popular techniques provide approximations of very low exceedance probabilities with very few calls to the model. But no confidence interval is estimated to validate the geometrical approximations.

Finally, an alternative technique is to use a given budget of model runs to build a surrogate model $\tilde{G}(\cdot)$ which requires negligible CPU time for subsequent runs. Monte Carlo is then performed on $\tilde{G}(\cdot)$ instead of $G(\cdot)$. Many techniques are provided in the Open TURNS package, among them the polynomial chaos expansion (PCE) [28] and the kriging approach [29].

The analyst is invited to mix methods and optimize an evaluation strategy with respect to a calculus budget. The validation comes from the confrontation of results obtained by different methods.

2.5 Step C' - Uncertainty Importance Ranking

The ranking of the uncertainty sources is based on the evaluation of some importance factors, correlation coefficients and sensitivity factors, the choice of which varies according to the quantities of interest specified in Step A. See [30] for an introductory overview of the problem.

In central dispersion studies, the Sobol's indices explain the variability of the outcomes by the variability of the input parameters or sets of parameters. Their evaluation by Monte Carlo sampling is costly and surrogate modeling approach (in particular PCE) are of great help. More simple correlation based indices (SRC, SRRC, PCC, PRCC indicators) could also be useful in practice.

In a threshold exceedance study, importance factors could be defined as particular Sobol indices after the linearization of the model around a specific point in the standard space. They quantify the impact of the global input uncertainty on the estimated exceedance probability.

According to the nature of the highest impact uncertainty source, feedback actions will differ: epistemic uncertainty requires some additional work to increase knowledge; reducible stochastic uncertainty requires some variability reducing actions; and irreducible stochastic uncertainty requires some modifications of the system in order to protect it against that unavoidable highest impact variability. These actions do not have the same consequences from the economical point of view, and do not address time equivalent issues.

3 The Open TURNS Software

3.1 An Open Source Software

Open TURNS [31] is an open source software package designed to implement the uncertainty framework sketched above. The package is distributed under LGPL and FDL licenses for the code source and its documentation respectively.

Running under the Windows and Linux environment, Open TURNS is a C++ library proposing a Python textual interface. It can be linked to any code communicating through input - output files (thanks to generic wrapping files) or to any Python-written functions. It also proposes standard interface for complex wrappings (distributed wrappers, binary data).

Gradients of the external code are taken into account when available and otherwise can be approximated automatically by finite differences schemes. In addition to its more than 40 continuous/discrete univariate/multivariate distributions, Open TURNS proposes several dependence models based on copulas: independent, empirical, Clayton, Frank, Normal, Gumbel, Sklar copulas. It offers a great variety of definitions of a multivariate distribution: list of univariate marginals and the copula, linear combination of probability density functions or random variables. Uncertainty propagation step is accomplished through numerous simulation algorithms. Open TURNS implements the innovative Generalized Nataf transformation and the Rosenblatt one for the FORM/SORM methods. For ranking analysis, Open TURNS implements the Sobol indices, in addition to the usual statistical correlation coefficients.

Open TURNS has a rich documentation suite comprising more than 1000 pages, dispatched within 8 documents covering all the aspects of the platform: scientific guidelines (Reference Guide), end-user guides (Use Cases Guide, User Manual and Example Guide) and some software documentations (Architecture Guide, Wrapper Guide, Contribution Guide and Windows port Guide).

Open TURNS implements select high performance computing capabilities such as the parallelisation of algorithms manipulating large data set (up to 10^8 scalars) using the threading building blocks technology (TBB). It also provides a generic parallel implementation of the evaluation of models over large data set using either pthreads or TBB.

3.2 Some Innovative Aspects

Open TURNS is innovative in several aspects. Its input data model is based on the multivariate cumulative distribution function (cdf). This enables the usual sampling approach, as would be appropriate for statistical manipulation of large data sets, but also facilitates analytical approaches. If possible, the exact final cdf is determined (thanks to characteristic functions implemented for each distribution, the Poisson summation formula, the Cauchy integral formula, ...). Furthermore, different sophisticated analytical treatments may be explored: aggregation of copulas, composition of functions from \mathbb{R}^n into \mathbb{R}^p , extraction of copula and marginals from any distribution.

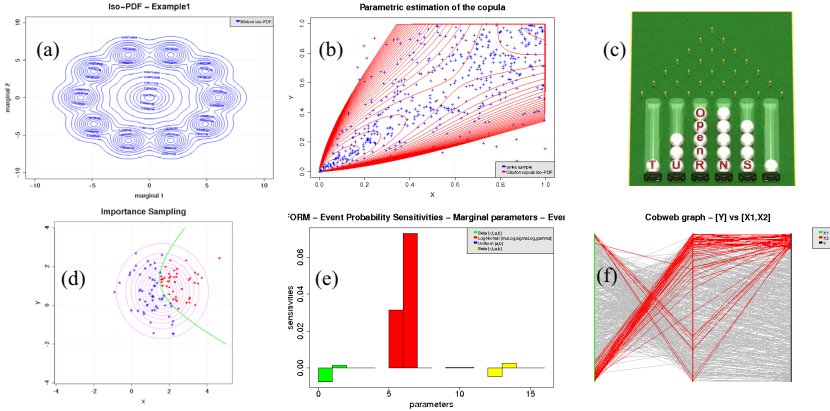


Fig. 1. Some Open TURNS snapshots: (a) the Open TURNS logo inspired by Galton’s box experience, (b) modeling a multi-modal random vector of \mathbb{R}^2 , (c) copula’s fitting, (d) importance sampling in the standard space around the FORM design point, (e) FORM importance factors, (f) cobweb plots

Open TURNS implements up-to-date and efficient sampling algorithms. The Mersenne Twister Algorithm is used to generate uniform random variables [32], the Ziggurat method for normal variables [33], the Sequential Rejection Method for binomial variables and the Tsang & Marsaglia method for Gamma variables [34]. Exact Kolmogorov statistics are evaluated with the Marsaglia Method and the Non Central Student and Non Central χ^2 distribution with the Benton & Krishnamoorthy method [35].

Open TURNS is the repository of recent results of PhD research performed at EDF R&D. In 2011, sparse PCE based on the LARS method [36] was implemented. In a future release the ADS (Adaptive Directional Stratification, [37]) accelerated Monte Carlo sampling technique will be made available for Open TURNS users.

4 Examples of Applied Studies

We sketch examples from applied studies excerpted from recent works performed at EDF R&D. Despite being representative of real industrial problems, these examples are provided for demonstration purposes only and the results cannot be used to draw any general conclusion about EDF risk assessment studies.

4.1 Flood Risk Assessment after the Failure of an Earth Dam

Considering that EDF is a major hydro-power operator (operating more than 200 dams and 400 power stations) and the role played by sea and river water in the nuclear power generation, it follows that hydraulic simulation is an important topic of interest for EDF R&D. In particular, most EDF studies are concerned with flood risk. As an example, a recent study [38] investigates the flood risk

assessment of a valley in the event that a dominating earth dam fails. Unlike concrete dams, which generally collapse and empty instantaneously, earth dam failure is assumed to be progressive and characterized by a so called *failure hydrograph*, i.e. a function $Q = H(t)$, describing the emptying discharge Q as a function of time t . Due to the complexity of the physics involved during the failure process, the precise shape of a hydrograph is not well known. Oft-used *ansatz* in these studies are that (i) the hydrograph has a triangular shape, (ii) the reservoir volume W at the beginning of the failure ($t = 0$) is known and (iii) the reservoir will completely empty during the observation period $[0, T_{obs}]$, i.e. $\int_0^{T_{obs}} H(t) \cdot dt = W$. Under these assumptions, the failure hydrograph is completely determined by the peak discharge Q_{max} and the time T_m at which the maximum discharge occurs.

The hydraulic modeling of the flood through the underlying valley is implemented by the MASCARET software [39] (resolution of 1D shallow water De St. Venant's equations) jointly developed by EDF R&D and CETMEF (Centre d'Etudes Techniques Maritimes et Fluviales). The geometrical features of the valley, here modeled as a 200 km long 1D channel (length, slope, section shape) are supposed to be known. On the other hand, the hydraulic friction parameter K_s (Strickler's coefficient) is uncertain and modeled as a random variable.

Three random variables are propagated through the hydraulic model: Q_{max} , T_m and K_s . The output variables of interest are the maximum water level Z_{max} reached by the wave front in the most dangerous points of the valley and the corresponding arrival time T_f . The two most dangerous points (located downstream a section narrowing, which gives rise to an hydraulic jump) have been previously identified by physical consideration. They are located 11 km (Point 1) and 60 km (Point 2) downstream from the dam, respectively.

The uncertainty propagation has been performed by first building a polynomial response surface, then Monte Carlo sampling. A sensitivity analysis has also been made to find out the most influential variables on Z_{max} and T_f in different points of the valley. The most interesting results of the study are: (i) the quantiles (95%, 99% and 99.9%) of Z_{max} in Points 1 and 2 and (ii) the Spearman ranks correlation coefficients between Z_{max} (T_f , respectively) and the three input random variables. As an example of results the 99% quantiles of Z_{max} in Points 1 and 2 are respectively 675.6 and 516.5 m above mean sea level (amsl). The analysis of Spearman's coefficients is particularly interesting. The most influential variable with respect to Z_{max} evaluation is the peak discharge Q_{max} . On the other hand, as far as T_f is concerned, it can be noticed that for the abscissas located close to the dam the most influential variable is T_m , but as one moves more and more downstream, the influence of Q_{max} and K_s raises. 90 km downstream from the dam, the friction coefficient becomes the dominant variable in the response evaluation.

This kind of study is valuable for supporting public powers in preparing the Emergency Response Plans in case of dam failure (e.g. planning evacuation of the most exposed areas). The sensitivity analysis is important to let the decision maker be aware of the weight of the hypotheses taken on the input variable and to possibly guide further study to reduce the uncertainties tainting the influential variables.

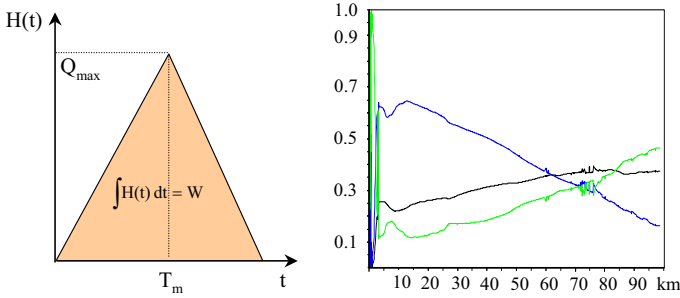


Fig. 2. Flood risk example [38]: hypothesis on the failure hydrograph (left) and sensitivity analysis by Spearman's ranks correlation coefficients (right) of T_f with respect to Q_{max} , T_m and K_s along the valley, up to 100 km downstream the dam

4.2 Globe Valve Sensitivity Analysis

EDF R&D has a deep history and experience in the application of uncertainty analysis methods in the field of solid mechanics. Many applied studies have been performed over the years, concerning for instance cooling towers, containment structures, thermal fatigue problems, lift-off assessment of fuel rods etc. We will focus on an application concerning reliability and sensitivity analysis of globe valves [40]. This investigation was one of the industrial case studies proposed by EDF in the context of the program, *Open Source Platform for Uncertainty Treatment in Simulation* (OPUS), funded by the French National Research Agency (ANR) between April 2008 and September 2011 [41].

Industrial globe valves are used for isolating a piping part inside a fluid circuit. This study is concerned with the mechanical behavior of the valve under water pressure. For this exemplary study, the variables of interest are the maximum displacement of the rod and the contact pressures. The tightness performance of the valve is assured if these variables stand below stated threshold values. The numerical model has been implemented thanks to the *Code_Aster* software, developed by EDF R&D and distributed under GPL license [42].

We will focus here on the sensitivity analysis of the maximum rod displacement Z . The problem has six uncertain input variables X_i , $i = 1 \dots 6$: packings, glands, beams, steel rod Young's modulus, hydraulic load and clearance. The goal of the study is the evaluation of Sobol's indices, which quantifies the contribution of each input X_i (or combinations of inputs, e.g. X_i and X_j) to the variance of the output $\mathbb{V}[Z]$:

$$S_i[Z] = \frac{\mathbb{V}[\mathbb{E}[Z|X_i]]}{\mathbb{V}[Z]}, \quad S_{ij}[Z] = \frac{\mathbb{V}[\mathbb{E}[Z|X_i, X_j]]}{\mathbb{V}[Z]} - S_i[Z] - S_j[Z] \quad \dots$$

In practice, the Monte Carlo evaluation of the variances of the conditional expectations above is unfeasible due to computational resource constraints. One path to resolve this problem is by implementation of a polynomial chaos expansion (PCE). This technique consists in replacing the random output of the

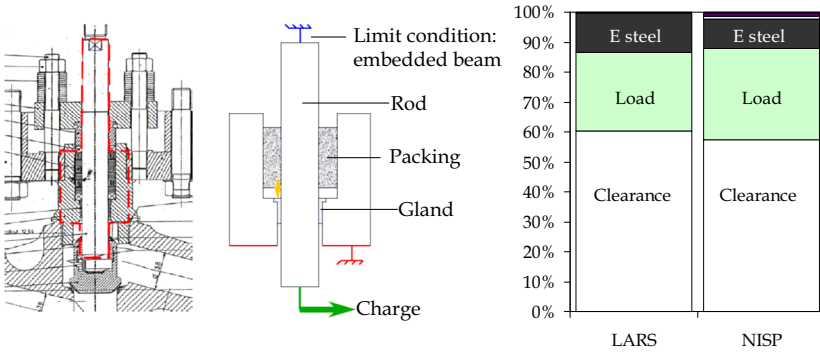


Fig. 3. Globe valve example [40]: cross sectional view (left), mechanical scheme (center) and Sobol's first order indices (right)

physical model by a decomposition onto a basis of orthonormal polynomials. The problem is reduced to the estimation of a finite set of coefficients, under the basis of a given number of previous runs of the physical model. As shown for instance in [43], once the coefficients have been determined, the evaluation of Sobol's indices is straightforward due to the orthonormality of the polynomials. PCE is particularly suited for this kind of problem.

Different methods have been tested for estimating the PCE coefficients. We have found that the LARS method [36] (cf. Section 3.2) and the NISP library (*Non Intrusive Spectral Projection*, developed by CEA [44]) return similar results, cf. Fig. 3.

5 Conclusion

Throughout this paper we have attempted to present an industrial perspective on UQ as we see it in our current practice. Of course, we do not pretend to provide an exhaustive nor prescriptive vision of this large problem.

Our approach is strictly non-intrusive and the problem is primarily viewed as a propagation of uncertainties from inputs to outputs of a numerical code. Some further steps for improving this methodology include: (i) systematically accounting for uncertainties tainting the computer model itself (the works carried by the MUCM [45], based on the Bayesian analysis of numerical codes [46,47] will be indeed of great help), (ii) linking of the common methodology sketched in Section 2 with decision theory, (iii) dealing with high dimension stochastic problems ($m \approx 100$) and (iv) treatment of functional inputs and outputs.

There can be no doubt that UQ is currently deeply rooted into EDF R&D practice. Our motivation for further work takes inspiration by our belief that industrial studies benefit from the consolidated practice of a common methodological framework and the Open TURNS software.

Acknowledgements. We gratefully thank the colleagues who worked on the industrial studies, sketched in Section 4 and in particular A. Arnaud,

M. Berveiller, G. Blatman and N. Goutal, as well as E. Remy and B. Iooss for their valuable advices. This work was partially supported by the French Ministry of Economy in the context of the CSDL project (*Complex Systems Design Lab*) of the Business Cluster System@tic Paris-Région.

References

1. Schweber, S., Wachter, M.: Complex Systems, Modelling and Simulation. *Stud. Hist. Phil. Mod. Phys.* 31, 583–609 (2000)
2. Heymann, M.: Understanding and misunderstanding computer simulation: The case of atmospheric and climate science - An introduction. *Stud. Hist. Phil. Mod. Phys.* 41, 193–200 (2010)
3. Sundberg, M.: Cultures of simulations vs. cultures of calculations? The development of simulation practices in meteorology and astrophysics. *Stud. Hist. Phil. Mod. Phys.* 41, 273–281 (2010)
4. Pilkey, O.H., Pilkey-Jarvis, L.: *Useless Arithmetic: Why Environmental Scientists Can't Predict the Future*. Columbia University Press, New York (2007)
5. Helton, J.C., Sallaberry, C.J.: Conceptual basis for the definition and calculation of expected dose in performance assessments for the proposed high-level radioactive waste repository at Yucca Mountain, Nevada. *Reliab. Eng. Syst. Safe.* 94, 677–698 (2009)
6. Helton, J.C., Hansen, C.W., Sallaberry, C.J.: Uncertainty and sensitivity analysis in performance assessment for the proposed repository for high-level radioactive waste at Yucca Mountain, Nevada. *Reliability Engineering & System Safety* (2011) (in press), doi:10.1016/j.ress.2011.07.002
7. Zheng, Y., Wang, W., Han, F., Ping, J.: Uncertainty assessment for watershed water quality modeling: A Probabilistic Collocation Method based approach. *Adv. Water Resour.* 34, 887–898 (2011)
8. Eckert, N., Naaïm, M., Parent, E.: Long-term avalanche hazard assessment with a Bayesian depth averaged propagation model. *J. Glaciol.* 56, 563–586 (2010)
9. Asserin, O., Loredò, A., Petelet, M., Iooss, B.: Global sensitivity analysis in welding simulations - What are the material data you really need? *Fin. El. Analys. Des.* 47, 1004–1016 (2011)
10. Hopfe, C.J., Hensen, J.L.M.: Uncertainty analysis in building performance simulation for design support. *Energ. Buildings* 43, 2798–2805 (2011)
11. Vernon, I., Goldstein, M., Bower, R.G.: Galaxy Formation: a Bayesian Uncertainty Analysis. *Bayes. Anal.* 5, 619–670 (2010)
12. Crucifix, M., Rougier, J.: A Bayesian prediction of the next glacial inception. *Eur. Phys. J. Special Topics* 174, 11–31 (2009)
13. Antoniadis, A., Helbert, C., Prieur, C., Viry, L.: Spatio-temporal prediction for West African monsoon. *Environmetrics* 23, 24–36 (2012)
14. Allard, A., Fischer, N., Didieux, F., Guillaume, E., Iooss, B.: Evaluation of the most influent input variables on quantities of interest in a fire simulation. *J. Soc. Franc. Stat.* 152, 103–117 (2011)
15. Baraldi, P., Pedroni, N., Zio, E., Ferrario, E., Pasanisi, A., Couplet, M.: Monte Carlo and fuzzy interval propagation of hybrid uncertainties on a risk model for the design of a flood protection dike. In: Berenguer, C., Grall, A., Guedes Soares, C. (eds.) *Advances in Safety, Reliability and Risk Management: ESREL 2011*. CRC Press, Leiden (2011)

16. O'Hagan, A., Buck, C.E., Daneshkhah, A., Eiser, J.R., Garthwaite, P.H., Jenkinson, D.J., Oakley, J.E., Rakow, T.: Uncertain judgements: eliciting expert probabilities. John Wiley & Sons, Chichester (2006)
17. Shannon, C.: A mathematical theory of communication. *Bell Syst. Tech. J.* 27, 379–423, 623–656 (1948)
18. Embrechts, P., Lindskog, F., McNeil, A.: Modelling dependence with copulas and applications to risk management. In: Rachev, S.T. (ed.) *Handbook of Heavy Tailed Distributions in Finance*, pp. 329–384. Elsevier, Amsterdam (2003)
19. Dutfoy, A., Lebrun, R.: A practical approach to dependence modeling using copulas. *Proc. Inst. Mech. Eng. O J. Risk Reliab.* 223, 347–361 (2009)
20. Lebrun, R., Dutfoy, A.: An innovating analysis of the Nataf transformation from the viewpoint of copula. *Probabilist. Eng. Mech.* 24, 312–320 (2009)
21. Del Moral, P.: *Feynman-Kac Formulae - Genealogical and interacting particle systems with applications*. Springer, New York (2004)
22. Lebrun, R., Dutfoy, A.: A generalization of the Nataf transformation to distributions with elliptical copula. *Probabilist. Eng. Mech.* 24, 172–178 (2009)
23. Lebrun, R., Dutfoy, A.: Do Rosenblatt and Nataf isoprobabilistic transformations really differ? *Probabilist. Eng. Mech.* 24, 577–584 (2009)
24. Rosenblatt, M.: Remarks on a multivariate transformation. *Ann. Math. Statist.* 23, 470–472 (1952)
25. Dolinski, K.: First-order second-moment approximation in reliability of structural systems: critical review and alternative approach. *Struct. Saf.* 1, 211–231 (1983)
26. Hasofer, A.M., Lind, N.C.: Exact and invariant second moment code format. *J. Eng. Mech.* 100, 111–121 (1974)
27. Tvedt, L.: Second order probability by an exact integral. In: Thoft-Christensen, P. (ed.) *2nd IFIP Working Conference on Reliability and Optimization on Structural Systems*, pp. 377–384. Springer, Berlin (1988)
28. Ghanem, R.G., Spanos, P.D.: *Stochastic Finite Elements: A Spectral Approach*, Revised Edition. Dover, Mineola (2003)
29. Sacks, J., Welch, W.J., Mitchell, T.J., Wynn, H.P.: Design and Analysis of Computer Experiments. *Stat. Sci.* 4, 409–435 (1989)
30. Saltelli, A., Tarantola, S., Campolongo, F., Ratto, M.: *Sensitivity analysis in practice: a guide to assessing scientific models*. John Wiley & Sons, Chichester (2004)
31. Open TURNS, Open Treatment of Uncertainties, Risk's and Statistics, an open source platform, <http://www.openturns.org>
32. Saito, M., Matsumoto, M.: SIMD-oriented Fast Mersenne Twister: a 128-bit Pseudorandom Number Generator. In: Keller, A., Heinrich, S., Niederreiter, H. (eds.) *Monte Carlo and Quasi-Monte Carlo Methods 2006*, pp. 607–622. Springer, Berlin (2006)
33. Doornik, J.A.: An Improved Ziggurat Method to Generate Normal Random Samples. Working paper, Department of Economics, University of Oxford (2005)
34. Marsaglia, G., Tsang, W.W.: The Ziggurat method for generating random variables. *J. Stat. Softw.* 5, 1–7 (2000)
35. Benton, D., Krishnamoorthy, K.: Computing discrete mixtures of continuous distributions: noncentral chisquare, noncentral t and the distribution of the square of the sample multiple correlation coefficient. *Comput. Stat. Data An.* 43, 249–267 (2003)
36. Blatman, G., Sudret, B.: Efficient computation of global sensitivity indices using sparse polynomial chaos expansions. *Reliab. Eng. Syst. Safe.* 95, 1216–1229 (2010)

37. Munoz Zuniga, M., Garnier, J., Remy, E., De Rocquigny, E.: Analysis of adaptive directional stratification for the controlled estimation of rare event probabilities. *Stat. Comput.* 22, 809–821 (2012)
38. Arnaud, A., Goutal, N., De Rocquigny, E.: Influence des incertitudes sur les hydrogrammes de vidange de retenue en cas de rupture progressive d'un barrage en enrochements sur les zones inondées en aval. In: *SimHydro 2010 Conference*, Sophia Antipolis (2010) (in French)
39. Goutal, N., Maurel, F.: A finite volume solver for 1D shallow-water equations applied to an actual river. *Int. J. Numer. Meth. Fl.* 38, 1–19 (2002)
40. Berveiller, M., Blatman, G.: Sensitivity and reliability analysis of a globe valve using an adaptive sparse polynomial chaos expansion. In: *11th International Conference on Applications of Statistics and Probability in Civil Engineering*, Zurich (2011)
41. OPUS Contributors: Final Report of the ANR OPUS project (2011), <http://www.opus-project.eu>
42. EDF R&D: Code_Aster, Analysis of Structures and Thermomechanics for Studies & Research, <http://www.code-aster.org>
43. Sudret, B.: Global sensitivity analysis using polynomial chaos expansions. *Reliab. Eng. Syst. Safe.* 93, 964–979 (2008)
44. Crestaux, T., Martinez, J.M., Le Maitre, O.: Polynomial chaos expansions for sensitivity analysis. *Reliab. Eng. Syst. Safe.* 94, 1161–1172 (2009)
45. MUCM: Managing Uncertainty in Complex Models, <http://www.mucom.ac.uk/>
46. O'Hagan, A.: Bayesian analysis of computer code outputs: a tutorial. *Reliab. Eng. Syst. Safe.* 91, 1290–1300 (2006)
47. Goldstein, M.: External Bayesian analysis for computer simulators. In: Bernardo, J.M., Bayarri, M.J., Berger, J.O., Dawid, A.P., Heckerman, D., Smith, A.F.M., West, M. (eds.) *Bayesian Statistics 9*, pp. 201–228. Oxford University Press (2011)

Discussion

Speaker: Alberto Pasanisi

Michael Goldstein: I consider the notion of a unified formulation across applications as natural and valuable. I wonder how the model discrepancy, i.e., the difference between the model and the system that the model tries to represent, is represented within the unified formulation.

Alberto Pasanisi: That is a crucial question and I thank Michael for giving me the opportunity to discuss our viewpoint. Actually, our general formulation of the problem and the methodological framework going with do not cope explicitly with model discrepancy. According to this scheme, UQ is mainly seen as the propagation of parametric uncertainties from inputs X to output Z of a deterministic computer model $Z = G(X)$. In some studies, generally concerning inverse problems (e.g. [1]), we did explicitly account for an additive Gaussian error in the observation model, so that $Z = G(X) + \epsilon$, but in most cases we simply consider the model, provided by the experts of given specific application fields as a black-box admitted *as is*. That is a purely pragmatic viewpoint, as in most cases the phases of verification & validation of the numerical code and parametric uncertainties propagation are made in separate times by different teams. In addition, a quite shared viewpoint in Uncertainty Analysis practitioners' community is that if the analyst does not trust enough the computer model, he/she must first improve it, before carrying an uncertainty and a (following) risk analysis [2].

Even if I acknowledge that the simplified framework I sketched makes thing easier in the engineering practice, I am aware of the limits of such a scheme and I hope that the use of more extended approaches quantifying both parametric and model's uncertainties will soon become a more standard practice in our studies. And I think that the work you carried with A. O'Hagan and your colleagues of MUCM will be of great help.

William Oberkampf: Model form uncertainty and, in many cases, model parametric uncertainty is epistemic (lack of knowledge) uncertainty. Epistemic uncertainty may be characterized as a probability distribution, but this represents incertitude as a random variable; which it is not. A more proper representation is to characterize incertitude as an interval-valued quantity, i.e. no knowledge structure over the range of the interval. This type of uncertainty analysis requires the use of a broader framework usually referred to as imprecise probability theory. Has EDF investigated the use of imprecise probability distributions in its uncertainty quantification?

Alberto Pasanisi: This question concerns a very important topic, namely, in a slightly reformulated way, "is the probabilistic assumption too informative for coping with purely epistemic uncertainties?" Actually, in our current practice, we use probabilistic modeling for both epistemic and stochastic uncertainty; indeed the Bayesian paradigm seems to give us a reasonable setting for coping with

both sources of uncertainties in a decisional framework. Nevertheless, we have also carried more perspective works involving Dempster-Shäfer Theory [3,4] or a *hybrid* framework [5] combining probabilistic and possibilistic modeling of uncertainties. The results about extra-probabilistic modeling are encouraging but, as far as we are concerned, some issues (e.g. modeling dependencies) still need to be investigated before these methods could be widely applied in engineering practice.

Jeffrey Fong: Is the failure envelope boundary line the result of a deterministic analysis, or, stochastic with a 95% lower limit? If the former, then the failure envelope is not uncertainty-quantification-based at all. Please clarify.

Alberto Pasanisi: As we do not tackle explicitly model's uncertainty in our current framework, the failure domain $\mathcal{D}_f := \{x; G(x) \geq z^*\}$ is deterministic: it is just the set of values of the input vector X that produce values of the output Z corresponding to failure conditions. So, the probability of failure is the probability for the random input X to belong to the failure domain \mathcal{D}_f .

Maurice Cox: In your framework for uncertainty management you referred to various principles. Such principles are set out in the GUM (Guide to the Expression of Uncertainty in Measurement) and Supplements to the GUM. Does EDF use these documents, or is this a parallel development by EDF?

Alberto Pasanisi: Yes, absolutely. Actually, our framework is largely inspired by the GUM (and its supplements) which is a reference document in EDF's practice. The GUM is widely used by EDF's engineers and technicians working in R&D and Engineering Departments, and in power plants.

Pasky Pascual: Maybe I misunderstood, but you seemed to suggest that Bayesian inference is a way to address the issue of imprecise probabilities. But doesn't Bayes assume well-described pdfs or at least probability distributions that can be (somewhat) estimated?

Alberto Pasanisi: I think that it was a misunderstanding. My idea was that Bayesian setting allows to take into account an additional level of uncertainty tainting the probabilistic distributions of inputs, and that this framework fits comfortably most industrial requirements. Of course, imprecise probabilities constitute a different way to address the problems.

Mark Campanelli: How does your framework do sensitivity analysis? In particular, is sensitivity analysis done prior to uncertainty analysis in order to determine which parameters can be treated as fixed? Furthermore, can these sensitivity analyses incorporate dependencies between random variables, and if so, how?

Alberto Pasanisi: According to our schematic framework, sensitivity analysis (SA) is performed at the same time than uncertainty propagation. That happens, for instance, when putting into practice advanced method of SA, as Sobol's decomposition of the output's variance. Nevertheless, in particular when the

number of inputs is large it is recommended to perform, prior to uncertainty analysis a first SA with less costly techniques (e.g. screening [6] or Morris method [7]) which, even if based on simplified assumptions, provides a first selection of influent variables. Then fixed values are given to less influent variables, thus reducing the stochastic dimension of the problem. Cf. also [8] for a pragmatic approach to the choice of the SA method, depending on the context of the study. The second part of the question is much more tricky and concerns more advanced research works than industrial R&D practice. In engineering studies, the most pragmatic way for coping with this problem is to gather dependent variables in groups and evaluate sensitivity indices for each one of these groups. Moving to more advanced works, you can see [9] for an introduction to the problem. That is a quite active research topic. Recent interesting papers concerned with this problem proposes several different approaches. In the linear case, Xu & Gertner [10] distinguish two indices, quantifying the contribution of a parameter due to its correlation with the other parameters and the contribution due to its own effect. In the non-linear case, Li et al. [11] propose a technique for the covariance decomposition and three types of Sobol's indices. Other works propose indices based on the distance [12] between the actual pdf of the output and conditional densities. These indices can be used in presence of correlated inputs, but their interpretation could not be easy. Finally techniques based on the copulas' formalism are proposed by Kucherenko et al. [13].

Wayne King: Could you describe EDF needs in life extension and life prediction as it relates to reactors?

Alberto Pasanisi: That is an interesting and actually very wide question. I will give hereby some elements, focused on the key topic "running safely nuclear power units in the long-term" [14]. EDF operates today 58 pressurized water reactor units with three different power levels: 900 MW (34 units), 1300 MW (20 units) and 1500 MW (4 units). Nuclear generation represents about 85% of EDF power generation. EDF nuclear power plants were designed for operating during 40 years at least. The lifespan of some components is supposed to be greater than 40 years, while others must be replaced before, e.g. transformers should be replaced after 25-30 years. As another example, the EDF Board has approved in September 2011 an order for 44 steam generators, for its 1300 MW units.

The mean age of EDF power units is around 29 years: most of nuclear reactors operating worldwide are contemporary or older than EDF's ones. Nowadays, according to international studies lead on both lifespan and maintenance policies of several nuclear units in different countries, the target of 60 years lifespan is considered to be granted, by a technical point of view. Since several years, EDF sets the technical conditions to operate its nuclear unit well beyond 40 years: components' refurbishing and replacing programs currently run and will continue in the next years. The extension of the lifespan will have to meet the compliance with specific safety objectives which will be fixed by the French Regulation Authority (ASN). By its side, the strategy of EDF for assuring a safe and high performance running of its units in the long term is based on the five pillars below:

- The ten-yearly inspection of each unit. Under the control of the Regulation Authority, it is actually a complete check-up of the unit's facilities. With a duration of about 90 days, this exceptional shutdown period allows to realize a huge number of controls and maintenance works. As a matter of facts, the safety level of each unit is then reinforced every ten years. After the end of the inspection, the Regulation Authority gives its verdict about the continuation of the unit's operation for ten more years.
- The modification and the refurbishing of unit's devices. These operations are lead regularly and can take place during ten-yearly inspection or other shutdown periods. Thanks to the technical similarity of EDF's units, these works take profit of technological advances and the enhanced feedback of the whole nuclear fleet.
- The survey and the anticipation of equipment's ageing. EDF has set an ambitious maintenance policy of its components. Depending on the features and the role played by each equipment, the maintenance policy could be scheduled, condition-based or corrective. Other actions as long-term partnership with subcontractors to avoid technical obsolescence or shortage problems complete this set of actions. As a key figure, EDF spends yearly about 2 billions of euros for the maintenance, refurbishing and modification of nuclear units' equipment.
- The preservation and the renewal of human skills. Nuclear units' operation needs workers with very specific and high skills. As a significant part of technicians and engineers working in nuclear units will retire in the very next years, this question is crucial and challenging and several actions have already been set by HR to cope with (e.g. recruitment campaigns, tutoring, partnerships with universities and engineering schools).
- The improvement of technical and technology knowledge. With its large staff and budget (around 2000 people and 486 millions of euros in 2010 respectively [15]), EDF R&D has a key role in this action. R&D activities cover all disciplinary fields involved in nuclear process. As an example, two recently acquired equipments of EDF R&D: the TITAN Transmission Electron Microscope and the IBM Blue Gene super-computer witness the ambition to enhance more and more the knowledge of components and materials of nuclear units, by both physical and computer experiments.

References

1. Celeux, G., Grimaud, A., Lefebvre, Y., De Rocquigny, E.: Identifying intrinsic variability in multivariate systems through linearised inverse methods. INRIA Research Report RR-6400 (2007)
2. Aven, T.: Some reflections on uncertainty analysis and management. *Reliab. Eng. Syst. Safe.* 95, 195–201 (2010)
3. Limbourg, P., De Rocquigny, E.: Uncertainty analysis using evidence theory – confronting level-1 and level-2 approaches with data availability and computational constraints. *Reliab. Eng. Syst. Safe.* 95, 550–564 (2010)

4. Le Duy, T.D., Vasseur, D., Couplet, M., Dieulle, L., Bérenguer, C.: A study on updating belief functions for parameter uncertainty representation in Nuclear Probabilistic Risk Assessment. In: 7th International Symposium on Imprecise Probability: Theories and Applications, Innsbruck (2011)
5. Baraldi, P., Pedroni, N., Zio, E., Ferrario, E., Pasanisi, A., Couplet, M.: Monte Carlo and fuzzy interval propagation of hybrid uncertainties on a risk model for the design of a flood protection dike. In: Berenguer, C., Grall, A., Guedes Soares, C. (eds.) *Advances in Safety, Reliability and Risk Management: ESREL 2011*. CRC Press, Leiden (2011)
6. Campolongo, F., Tarantola, S., Saltelli, A.: Tackling quantitatively large dimensionality problems. *Comput. Phys. Commun.* 117, 75–85 (1999)
7. Morris, M.: Factorial sampling plans for preliminary computational experiments. *Technometrics* 33, 161–174 (1991)
8. De Rocquigny, E., Devictor, N., Tarantola, S. (eds.): *Uncertainty in Industrial Practice*. Wiley, Chichester (2008)
9. Kurowicka, D., Cooke, R.: *Uncertainty analysis with high dimensional dependence modelling*. Wiley, Chichester (2006)
10. Xu, C., Gertner, G.Z.: Uncertainty and sensitivity analysis for models with correlated parameters. *Reliab. Eng. Syst. Safe.* 93, 1563–1573 (2008)
11. Li, G., Rabitz, H., Yelvington, P.E., Oluwole, O.O., Bacon, F., Kolb, C.E., Schoendorf, J.: Global Sensitivity Analysis for Systems with Independent and/or Correlated Inputs. *J. Phys. Chem.* 114, 6022–6032 (2010)
12. Borgonovo, E.: A new uncertainty importance measure. *Reliab. Eng. Syst. Safe.* 92, 771–784 (2007)
13. Kucherenko, S., Munoz Zuniga, M., Tarantola, S., Annoni, P.: Metamodelling and Global Sensitivity Analysis of Models with Dependent Variables. In: *AIP Conf. Proc.*, vol. 1389, pp. 1913–1916 (2011)
14. EDF Group: Exploiter les centrales nucléaires dans la durée (in French). Information Note (2011), <http://energie.edf.com/nucleaire/publications/notes-d-information-46655.html>
15. EDF Group: 2010 Activity and Sustainable Development Report (2011), <http://www.edf.com/html/RA2010/en/>