Towards intelligent methodologies for uncertainty quantification in civil nuclear energy safety

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Abstract: Redundancies and physical separation of safety systems are used in nuclear systems in order to cope with potential component failures, extreme events and threats all characterised by large uncertainties. Such uncertainties are unavoidable as they arise from, for instance, manufacturing tolerances, modelling capabilities, and sparsity in data (e.g. one-of-a-kind system, failure data), external and uncontrollable factors, etc. Historically, uncertainties in nuclear sector have been treated in a highly conservative manner, with large, inefficient margins to failure. Quantifying the effect of the uncertainty is essential for ensuring the safety of nuclear installations and also for supporting the lifetime economic viability of new nuclear power plant in design, building, operation and decommissioning. In fact, a proper quantification and propagation of uncertainty across multi-physical components allows to determine vulnerable components, prioritise investments, identify operational margins and adopt relevant measures to guarantee safety whilst reducing the overall cost of advanced nuclear design. Conventionally uncertainty quantification was limited to semi-analytical approaches and required strong assumptions (e.g. Gaussianity) due to the unmanageable computational costs of full probabilistic assessments posing serious question on the validity of the results. Such traditional methods, which are far from optimised, often lack a rigorous process for propagation of uncertainties, normally resulting in over-engineering. Recent advances in intelligent computing brings inspiration of new perspectives and analytics in the way we design, build, operate and decommission our systems. This paper presents an overview of the state-of-the-art methodologies and tools for managing and quantify uncertainty in nuclear systems.
Keywords: Digital Twin, Uncertainty quantification, Imprecise Probability, Nuclear safety.

1. INTRODUCTION

Historically, the treatment of uncertainties in nuclear analysis methods has been treated in a highly conservative manner, with large, inefficient margins to failure. Quantifying the effect of the uncertainty is essential for ensuring the safety of nuclear installations and also for supporting the lifetime economic viability of new nuclear power plant in design, building, operation and decommissioning. Historically uncertainty quantification was limited to semi-analytical approaches and used of strong assumptions (e.g. Gaussianity) due to the unmanageable computational costs of a full probabilistic assessment. Such traditional methods, which are far from optimised in the development of nuclear components, often lack a rigorous process for propagation of uncertainties, normally resulting in over-engineering. Recent advances in intelligent computing brings inspiration of new perspectives in the way we design, build, operated and decommission our systems.

An enhanced strategy is to take various uncertainties well into account and, at the same time, replace High-Fidelity models with data-supported simpler models (surrogate models) that can be combined with Uncertainty Quantification (UQ). Therefore, the joint use of surrogate models and UQ methods offers a potential solution, as it addresses engineering problems in a cost-effective and technically viable manner. The crucial point is to ensure a comprehensive and accurate UQ. Additionally, the novel opportunities that Artificial Intelligence seem to offer in the domain pose specific challenges: (1) Ensuring accurate data for AI/ML techniques; (2) Estimating AI/ML technique prediction uncertainties; (3) Exploring AI/ML compliance with standards and regulations.

This paper is organised as follows: a brief overview of the treatment of uncertainty in nuclear safety risk assessments is presented in Section 2, outlining the incentives for the eMEANSS project which aims to enhance the existing safety analysis and optimisation methodologies. It includes an exposition of the different types of uncertainty contributing to nuclear safety and the various sources from which they arise, the challenges in uncertainty modelling for a highly complex system such as a nuclear reactor. Section 3 summarises the state-of-the art computational techniques putting specific focus on trustful predictive modelling, imprecise probability and digital twin.

1.1. Enhanced Methodologies for Advanced Nuclear System Safety (eMEANSS) project

Uncertainties are unavoidable and complex systems such as nuclear reactors are designed to cope with them. Improper approaches, say considering individual worst cases scenarios without dependencies, would likely produce over-designed and expensive systems (i.e. conservatism) without guaranteeing their overall safety. By contrast, proper quantification and propagation of uncertainty across multi-physical components allows one to determine vulnerable componentry, prioritise investments, identify operational margins and adopt relevant measures to guarantee safety whilst at the same time reducing the overall cost of advanced nuclear design. Therefore, a re-assessment of the impact of uncertainties within the nuclear industry is of paramount importance, not only ensuring the continued safety of nuclear energy systems, but also to ensure the economic viability of new nuclear power plant design, build, operation and decommissioning.

2. UNCERTAINTY IN NUCLEAR ENGINEERING

Safety analyses are conducted to ensure that the design and operational controls of a nuclear facility provide assurance that the public, staff, and the environment are protected from all nuclear hazards. Owing to insufficient knowledge and understanding, conservatisms are introduced throughout the safety analyses (e.g. in acceptance criteria, assumptions of models, input conditions), such that the assurance of adequate protection can be provided, supporting disciplines (e.g., quality assurance) and design provisions (e.g. in-corporation of defense-in-depth and appropriate safety margins) and operational controls. Nuclear power technology has been developed based largely on the traditional defence-in-depth philosophy for the design of the plant that was supported by deterministic and overly conservative methods for safety analysis. In the past, large uncertainties in the computer models used for nuclear power system design and licensing have been compensated using highly conservative assumptions. Accident scenarios are typically assessed using worst case scenarios. Best estimate plus uncertainty (BEPU) is the leading methodology in validating existing safety margins, but it remains a challenge to develop and license such approaches.

2.1. Progress on nuclear safety assessment

Historical progress for the licensing approach have gone through a few phases: (I) Highly Conservative. (II) Realistic Conservative; and (III) Use of Best-Estimate Plus Uncertainty (BEPU) [1]. Initially conservative hypotheses were introduced for safety analyses to address existing uncertainties. Conventional engineering is using safety margins in design in order to compensate for the uncertainty in modelling and simulation, which typically assumes worst-case scenarios, intentional overestimation of parameters, and results in overdesign. This deterministic method, besides being costly, provides no way to estimate risk or determine failure probability and, thus, requires the use of heuristic safety factor in an attempt to avoid failures. With highly conservative assumptions, large uncertainties in the computer models used for nuclear power system design have been compensated. The Loss-Of-Coolant-Accident Evaluation Model is one of the main examples about this approach. The use of multiple conservative hypothesis can inflate to extremely conservative results but it is claimed that a reasonable degree of conservatism must be sought in nuclear safety analyses to strike the balance between safety and cost. In the absence of full propagation of parameter uncertainties, the use of mean values is consistent with the reasonable conservatism [2].

BEPU requires replacing subjective judgments about the inadequacy or the degree of conservatism in the assumptions with quantitative measures, which entails the propagation of code input uncertainty (selected number of parameters) through the code to obtain the output uncertainty (e.g. probability distribution function) either via code-nodalisation or repeated code runs [3, 4, 5]. A conceptual comparison, in terms of pros and cons, between the conservative and BEPU approaches can be found in [1].

Public concerns of nuclear safety and wider acknowledge of uncertainties leads to probabilistic frameworks in the management of uncertainty and risks of regulatory decision in the safety assessment. Probabilistic risk assessment (PRA), as set out in the Rasmussen Report [6], involves defining a system failure for complex multicomponent, multiphysics problems, identifying basic events that can cause a system failure, building a fault tree to relate component events to a system failure, and relating the joint probability of events to the probability of a system failure. It usually has a goal to mitigate the risk of nuclear safety decisions in the presence of uncertainty, through a comprehensive framework of calibration and the aggregation of risk information from various sources, including numerical calculations, expert opinions, risk attitudes, regulatory compliance, etc. [7, 8].

2.2. Challenges and recent developments on the characterisation and quantification of uncertainty

There presents many challenges in attempting to appropritely modelling the uncertainty, such as the understanding and modelling of the complicated physics in terms of a coupled multiphysical and nonlinear system that is numerically hard to solve, the increasing needs of power production constrained by the initial safety design limits on the basis of generally conventional conservatism tools, etc. Notably, a substantial challenge associated with uncertainty quantification for nuclear reactor designs is the necessity for propagating uncertainties through several linked simulation codes for all of the coupled subsystems. Heat transfer, coolant flow, neutron distributions, and fission reaction rates are all tightly coupled to form a highly complex multicompound, multiphysics system. The resulting models and simulation codes are computationally intensive per se, and it is compounded by the needs for comprehensive characterisation of uncertainty along the pipeline to confidently describing the quantity of interest (QoI).

Nevertheless, UQ remains an active area of research in reactor physics/analysis and many other sub-fields. [9] applied Total Monte Carlo methodology for nuclear data uncertainty propagation for fusion neutronics calculations and a number of fusion shielding benchmarks. A review of UQ application for computational fluid dynamics (CFD) analyses to nuclear reactor thermal hydraulics can be found in [10] and [11]. [12] investigates the measurement uncertainty based on the power monitoring data of a MIT research reactor (MITR-II). [13] proposes a new method that characterises imprecise and vague knowledge for detecting abnormal component of the system under uncertainty from the instrument and control system of nuclear plant system.

2.3. Source of uncertainty

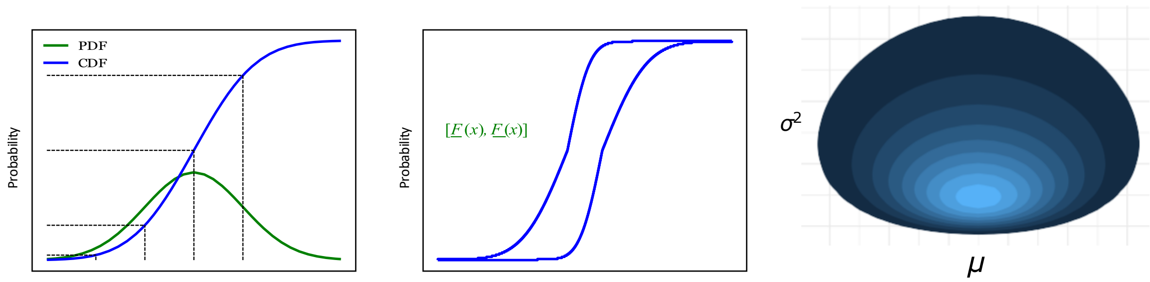
Uncertainties arise in many aspects of nuclear reactor system modelling: in the nuclear data, in the core geometry, in the simulation methods, and in the plant data with which simulation results are compared, etc. Generally those can be categorised into several sources of uncertainties and errors: input parameter uncertainties, model errors, numerical errors, and data uncertainties (measurement imprecision, sparse and even incomplete observations) [9, 14, 15]. Particularly, in developing tools and procedures for nuclear emergencies, [16] identifies 9 types of uncertainty: aleatoric, epistemic, actor, judgemental, computational, model uncertainty as well uncertainties related to ambiguity and lack of clarity, value, social and ethical aspects, and finally uncertainty about the depth of modelling.

In practice, limited plant data is available for both validating computational models and determining the relative contributions to overall uncertainties in such observations. Nuclear data evaluations would statistically mix experimental reaction data with reaction models to produce the best estimate of the nuclear data quantities plus uncertainty. However, due to the difficulty and cost of conducting nuclear reaction experiments, experimental data is often sparse or not present for the vast majority of nuclides and reactions. Excluding the main fission related nuclides, which have been extensively studied and have low uncertainties, the uncertainty may be severe for most nuclides, with the worst case being that the covariance information is completely missing in some evaluations [17].

The vision for a robust safety assessment workflow starts from a systematic approach towards nuclear data evaluation, in which uncertainties are taken into account in an appropriate way, and which relies on efficient high-fidelity nuclear reaction models (to be developed) and high-precision measurements (to be performed) [9]. The current imperfections with respect to the aspects above (nuclear physics experiments, models and parameters) drive the needs to appropriately account for the various sources of uncertainty for increasing overall confidence in nuclear safety.

2.4. Modelling uncertainty

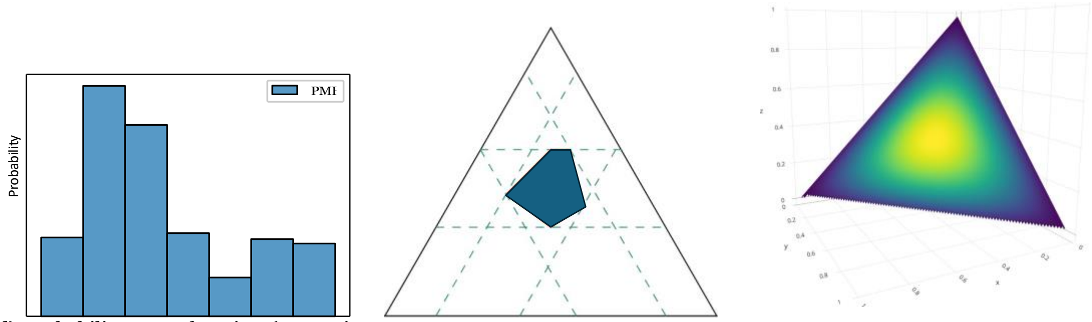
aleatory uncertainty addresses inherent variability in systems that cannot be eliminated even with com- plete knowledge. Also known as irreducible uncertainty, aleatory uncertainty is attributed to inherent randomness or variability in natural phenomena. epistemic uncertainty deals with uncertainties arising from incomplete knowledge or lack of information about a system. This type of uncertainty is often con- sidered reducible through additional data collection, research, or improved modelling techniques. While probability theory has been used as the orthodox tool for aleatoric uncertainty, there are more discussions and theories as to formulating epistemic uncertainty via non-probabilistic approaches [18, 19], which entails using intervals [20] and fuzzy variables [21] and seeks to narrow down uncertainty ranges by updating mod- els as new information becomes available. It plays a crucial role in refining prediction ranges and making informed decisions by continuously improving our understanding of uncertain factors. Particularly, mixed uncertainty model has attracted significant attention in recent years through the developments of generalized probability theories (i.e., imprecise probability, Dempster–Shafer theory) [20, 22], where uncertain numbers (with typical examples such as probability boxes and credal sets) play a foundational role in many modern risk assessments for complex engineering systems [23]. By comparison, hierachical Bayesian methods (the second-order distribution) also represent mixed type of uncertainty but uses probability distribution to ac- count for the uncertainty on shape parameters. Fig. 1 illustratively displays these models (primitives) for representing uncertainty.



(a) probability distribution (gaussian)

(b) probability box

(c) higher-order distribution (Gaussian inverse gamma)



(d) probability mass function (categorical) (e) credal sets (f) higher-order distribution (Dirichlet)

Figure 1: An illustration of the mathematical objects (primitives) representing uncertainty

2.5. Propagate uncertainty

Complex engineering systems such as nuclear reactor exhibit rich uncertainty from various components and hierarchies. Modern risk analyses of complex systems carefully distinguish aleatoric and epistemic uncertainty (also referred to as variability and incertitude). There are therefore challenges in the uncertainty analysis, at a system level, to represent, aggregate, and propagate mixed uncertainty types. The Monte- Carlo (MC) simulation may serve as one of the most widely used methods to propagate aleatory uncertainty. With MC it is possible to treat the model under study as a black box, enabling non-intrusive uncertainty propagation to be performed in abundant research and application domains. However, it is worthy to mention that such versatility generally comes at the cost of intensive computations for a nonlinear and high-dimensional complex system due to its brute-force nature [24]. With this said, the progress of efficient MC variants should also be well recognised [25]. Alternatively, interval propagation is appealing as it can rigorously capture the uncertainty in QoI by yielding bounds via interval arithmetic. But its applicality presents a challenge due to the lack of open-source code numerical codes in simulations. When a mixture of aleatory and epistemic uncertainty is present in the input, characterised by second-order distributions or p-boxes, a number of different modifications have been proposed, including double-loop Monte-Carlo, generalized importance sampling and interval Monte Carlo [26].

One of the key challenges in delivering risk-based design optimisation for a multiphysics system is the computational burden through high-fidelity numerical simulations, coupled by the consideration of uncertainty. An efficient way to alleviate such burden is surrogate models which serve as efficient substitutes, capturing the underlying relationships between input and output variables in a non-intrusive fashion. By building a surrogate model, which is a simplified mathematical representation of the original model, one can significantly reduce computational costs while maintaining a reasonable level of accuracy. Surrogate Models are particularly useful for optimisation, sensitivity analysis, and uncertainty quantification tasks. In considering mixed aleatory-epistemic uncertainty quantification, which is highly challenging for complex numerical codes, [27] proposed to propagate probability boxes through interval predictor models. [28] deals with the propagation of uncertainty in the input parameters characterised as probability boxes through a deterministic, black-box computational model. Furthermore, two non-intrusive uncertainty propagation approaches are proposed in [29] for the analysis of generic engineering systems subject to interval uncertainties.

3. TOWARDS AUTONOMOUS DIGITAL TWINS FOR NUCLEAR SYSTEMS: UNCERTAINTY, DATA AND AI

Recent advancements in digitalisation and AI analytics offer novel and promising perspectives for modernised approaches to challenges and visions in nuclear uncertainty quantification and design optimisation. Notably, Digital Twins (DT) offer the possibilities of connecting the virtual and physical worlds to oversee the performance of an asset, identify potential faults and support better-informed decisions. Nuclear DT has been built to accelerate the development and deployment of advanced nuclear technology in areas of passive safety, new fuel forms, instrumentation, and reactor control [30], demonstrating potentials in applications of predictive maintenance, autonomous nuclear reactor control system, conceptual design optimisation, and improved project management, nuclear fuel manufacturing, etc [31]. With the built physical asset, the DT collect real-

time data, e.g. from smart sensors, to understand the status, monitor the health of the system, predict future scenarios and improving the fidelity of the simulation by dynamically updating the DT based on evidence.
DT represents an integrated framework for calibration, data assimilation, uncertainty-informed decision-making, planning and control, through, for instance, a probabilistic graphical model [32]. It dynamically updated asset-specific computational models integrated within the data-driven analysis and decision-making feedback loop [32]. The digital twin acquires and assimilates observational data from the asset (e.g., data from sensors or manual inspections) and uses this information to continually update its internal models,
e.g. Deep Learning (DL) models, so that they reflect the evolving physical system, which embodies a synergistic multi-way coupling between the physical system, the data collection, the computational models, and the decision-making process. One of the significant challenges is the uncertainty quantification [33, 34] which ranges from to errors in machine-learning models and low-quality sensors, uncertainties introduced by simulations, data, and machine learning surrogate models.

3.1. Predictive modelling with uncertainty awareness

The effectiveness of AI (e.g. DL) analytics have been widely recognised and utilised in the nuclear power industry chain to elevate data analyses and decision making at various steps such as nuclear fuel supply (upstream), nuclear equipment manufacturing (midstream), and the nuclear power plant design, operation, and maintenance (downstream) [35, 36, 37, 38].

However, data could be imperfect as being sparse, scarce, and imprecise. Learning from data of insufficient quality has restricted the effectiveness of data-driven techniques in learning the true underlying data generating process, which further degrades the performance of generalisation. It is required in many safety-critical applications or consequential engineering practices that the model should be capable of signalling when it is uncertain of its results (i.e. know when they do not know) to be robust and trustful, as opposed of over-confidently yielding inaccurate predictions/forecasts/decisions. Increasing attention has been therefore focused on the developments of Trustworthy AI which aims to critically investigate the fairness (biasness), interpretability, and robustness of Deep Learning algorithms and applications. Resorting to prior knowledge is an effective approach against data insufficiency, [39] proposes a meta-learning approach to robustly predict material properties for nuclear reactor design under limited data.

Imprecise probability framework further elevates the capacity of machine learning models in accounting for uncertainty, especially when dealing with partial or vague knowledge, such as when the available data is fairly limited such that a precise specification of probability density function (PDF) cannot be determined with confidence [40, 41, 42], or dealing with data incertitude (even in extreme cases as missing data) [43, 44, 45]. Importantly, IP enables the consideration of uncertainty in decision-making based on the predictive outcomes as it realistically characterises indecision where the current evidence is inadequate to yield a decision without over confidence.

Using AI analytics can also be beneficial in enhancing resilience and safety. Contrary to a human operator, AI systems could analyse huge amount of data and predict the consequences of the decision in critical situation without suffering from typical human related errors due to stress and environmental and organisational pressure [46]. Possessing the potential to enable autonomous control system (e.g. in nuclear power plants) [47], even as not implemented as fully autonomous, DT and AI can be used to pass only the most relevant information with clear level of “credibility” to a decision maker. AI can be employed to predicting potential malfunctions and autonomously making proactive decisions.

3.2. Tools and software coupling uncertainty quantification and deep learning

COSSAN a generalised software for uncertainty quantification in risk, reliability and resilience analy- ses [48, 49]. Probabilistic Programming Languages (PPL) that empowering a wide spectrum of Bayesian machine learning methods [50, 51, 52]

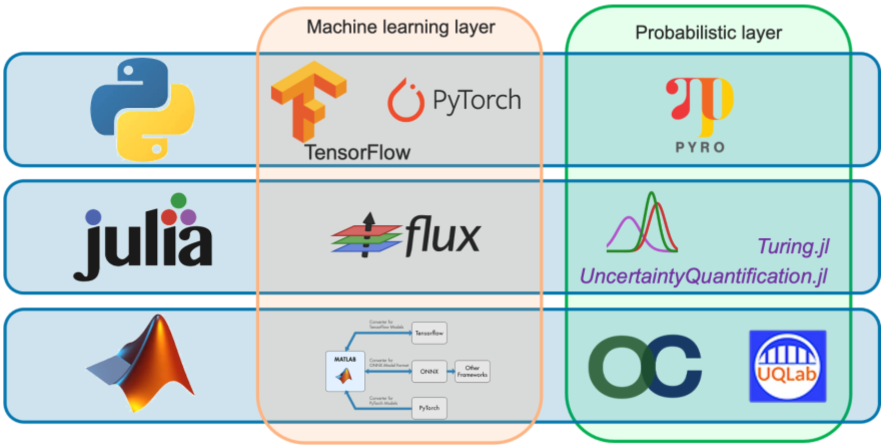


Figure 2. An overview of the programs and software coupling uncertainty quantification with deep learning

4. CONCLUSION

It has been widely recognised the needs for enhanced safety analyses and optimisation of nuclear systems to improve upon conservatism. Conventional conservatism cannot establish the safety margins in a quantitative manner neither achieve the optimisation of the safety solution. This paper sets out an enhanced strategy that leverages the state-of-the-art computing technologies, taking various uncertainties well into account, meanwhile, replacing High-Fidelity models with data-supported surrogate models (e.g. trustful Machine Learning (ML) models). This new strategy embodies a mutual coupling between the physical system, data collection, computational models, and the decision-making process. Notably, digital twin, as an emerging technology, serves as an integrated hub for calibration, data assimilation, uncertainty-informed decision-making, planning and control. Imprecise probability provides a rigorous representations of various uncertainties, including variability, imprecision, and vagueness, to be combined and expressed by the unified mathematical structure. The combination of ML and IP therefore leads to an elevated level of credibility where reliable decision can be based upon. By connecting the virtual and physical worlds, Digital twins offer the possibilities of to robustly oversee the performance of an asset, identify potential faults and support better-informed decisions. The enhanced strategy, coupled with the expertise from multidisciplinary and multi physical perspectives, has huge potentials to address critical challenges in verification, validation, and uncertainty quantification for the safe and confident use of digital twin technologies in advanced reactors.

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