Nuclear Engineering and Design 313 (2017) 29–52

Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes

Inverse uncertainty quantification of reactor simulations under the Bayesian framework using surrogate models constructed by polynomial chaos expansion

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ARTICLE INFO

Article history:
Received 13 May 2016
Received in revised form 14 November 2016
Accepted 28 November 2016

ABSTRACT

Modeling and simulations are naturally augmented by extensive Uncertainty Quantification (UQ) and sensitivity analysis requirements in the nuclear reactor system design, in which uncertainties must be quantified in order to prove that the investigated design stays within acceptance criteria. Historically, expert judgment has been used to specify the nominal values, probability density functions and upper and lower bounds of the simulation code random input parameters for the forward UQ process. The purpose of this paper is to replace such ad-hoc expert judgment of the statistical properties of input model parameters with inverse UQ process. Inverse UQ seeks statistical descriptions of the model random input parameters that are consistent with the experimental data. Bayesian analysis is used to establish the inverse UQ problems based on experimental data, with systematic and rigorously derived surrogate models based on Polynomial Chaos Expansion (PCE).

The methods developed here are demonstrated with the Point Reactor Kinetics Equation (PRKE) coupled with lumped parameter thermal-hydraulics feedback model. Three input parameters, external reactivity, Doppler reactivity coefficient and coolant temperature coefficient are modeled as uncertain input parameters. Their uncertainties are inversely quantified based on synthetic experimental data. Compared with the direct numerical simulation, surrogate model by PC expansion shows high efficiency and accuracy. In addition, inverse UQ with Bayesian analysis can calibrate the random input parameters such that the simulation results are in a better agreement with the experimental data.

1. Introduction

Mathematical modeling and computer simulations have long been the central technical topics in practically all branches of science and technology, from academia to industry. They are naturally affected by a relatively large amount of uncertainty in the input data such as model parameters, forcing terms, boundary conditions, and geometry. Confidence in modeling and simulation must be critically assessed which requires model Verification and Validation (V&V) (Oberkampf and Roy, 2010). Verification is the process to determine that the implementation of the model accurately represents the developer's conceptual description of the model and its solution. Validation is the process of determining the degree of accuracy of the considered model in representing real world physical phenomena.

The input data uncertainty can be included in the mathematical model by adopting a probabilistic setting, which requires enough information for a complete statistical characterization of the physical system, and the input parameters are then modeled as random variables. These input uncertainties may be characterized as either aleatory uncertainties (Cacuci, 2003), which are irreducible variabilities inherent in nature, or epistemic uncertainties, which are reducible uncertainties resulting from a lack of knowledge. Uncertainty Quantification (UQ) aims at determining the effect of such input uncertainties on response Quantity of Interest (QoI) and it plays a vital role in the validation process. See (Cacuci, 2003; Cacuci and Ionescu-Bujor, 2004; Ionescu-Bujor and Cacuci, 2004; Cacuci and Ionescu-Bujor, 2010) for a complete review. In nuclear reactor system design, uncertainties must be quantified in order to prove that the investigated design stays within acceptance criteria.

The importance of UQ-supported modeling and simulation continues to grow in the 21st century nuclear engineering, which faces the increasingly stringent demand for risk-informed safety margin characterization and plant performance optimization. This demand has intensified due to the fact that the licensing of nuclear installations has shifted from conservative to Best Estimate Plus Uncertainty (BEPU) methodologies (Wilson, 2013). Historically,

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http://dx.doi.org/10.1016/j.nucengdes.2016.11.032
0029-5493/

conservative approach calculates the output response of a code using extreme (unfavorable) values of input parameters. The reason for this approach is to model the physical phenomena such that it always predicts the worst case scenario. Consequently, conservative approach leads to considerable inaccuracy in Modeling and simulation. For example, it consistently over-estimates the cladding temperature and hence under-predicts the time to cladding failure.

UQ can be broadly classified as forward UQ and inverse UQ, as shown in Fig. 1. Forward UQ is the process of quantifying the uncertainties in QoIs by propagating the uncertainties in input parameters. It requires knowledge in the model or code input uncertainties, for example, the mean, variance, Probability Density Function (PDF), upper and lower limit, etc. The inverse UQ is the process of quantifying the uncertainty in input parameters given relevant experimental measurements and code simulation results (Shrestha and Kozlowski, 2015). Inverse UQ aims to quantify the uncertainty in input parameters such that the discrepancies between code output and observed experimental data can be minimized. In that sense, it is similar to parameter calibration or parameter estimation. However, unlike parameter calibration, inverse UQ also captures the uncertainty in its estimates rather than merely determining point estimates of the best-fit input parameters. The purpose of inverse UQ, and this paper, is to seek statistical descriptions of the code input model parameters that are consistent with the observed data.

Well-established approaches for performing UQ analysis can be categorized as deterministic methods which are typically based on perturbation theory, and statistical methods based on Monte Carlo (MC) sampling. They all require knowledge of uncertainty in the input parameters. Historically, the expert judgment has been used to specify the nominal values, PDFs and upper and lower bounds of code input parameters. Such ad-hoc description of statistical parameters and PDFs for code inputs is unscientific and lacks mathematical rigor, even if it has been considered reasonable for a long time. The purpose of this paper is to replace such ad-hoc expert judgment of the statistical properties of input model parameters in nuclear reactor simulation.

Previous research for inverse UQ (or similarly, statistical calibration) in nuclear engineering simulation including (Shrestha and Kozlowski, 2015; Hu and Kozlowski, 2016), in which a mathematical framework was developed where Expectation-Maximization (EM) algorithm was implemented to quantify input model parameter uncertainty using the Maximum Likelihood Estimate (MLE) and Maximum a Posteriori (MAP) estimate. However, these methods are limited by several restrictive assumptions: (1) the relation between the response and the input model parameter is assumed to be linear; (2) the input model parameters are assumed to follow a normal distribution; (3) local sensitivity analysis are required to provide the necessary input data for the MLE algorithm. Cacuci and Ionescu-Bujor (Cacuci and Ionescu-Bujor, 2010) developed a comprehensive mathematical framework for simultaneously calibrating model parameters and responses through the assimilation of experimental data, leading to best-estimate values with reduced uncertainties for both parameters and responses. This predictive modeling procedure was successfully demonstrated for large-scale, nonlinear, time-dependent systems (Petruzzi et al., 2010; Badea et al., 2012; Cacuci and Arslan, 2014; Arslan and Cacuci, 2014). This predictive modeling methodology has been demonstrated to be capable of significantly reducing the uncertainties of the best-estimate predicted results. Furthermore, recently an innovative mathematical methodology for "predictive modeling of coupled multi-physics systems (PMCMPS)" Cacuci, 2014 was developed by extending the predictive modeling methodology formulated in Cacuci and Ionescu-Bujor (2010) from a single physics system to coupled multi-physics systems. In (Cacuci and Badea, 2014; Latten and Cacuci, 2014) the PMCMPS method were demonstrated to yield best-estimate response and parameter values with reduced predicted uncertainties for each individual benchmark.

In the current research, we focus on Bayesian inference methods for inverse UQ. Bayesian method has been widely used for parametric uncertainty quantification and source inversion. Examples of applications range from geophysics (Malinverno, 2002), climate modeling (Jackson et al., 2004), heat conduction (Wang and Zabaras, 2004; Ma and Zabaras, 2009; Zabaras and Ganapathysubramanian, 2008; Kaipio and Fox, 2011) to groundwater reactive transport modeling (Zhang et al., 2013; Shi et al., 2014). A practical problem with Bayesian inference for inverse problems is the exploration of the posterior PDF by Markov Chain Monte Carlo (MCMC) sampling, during which a large number of model simulations are required. To deal with the large computational cost, various surrogate models based on stochastic spectral techniques have been used in inverse problems (Zhang et al., 2013; Shi et al., 2014; Marzouk et al., 2007; Marzouk and Xiu, 2009).

While an extraordinary progress was made during the past decade in developing advanced concepts and methods for

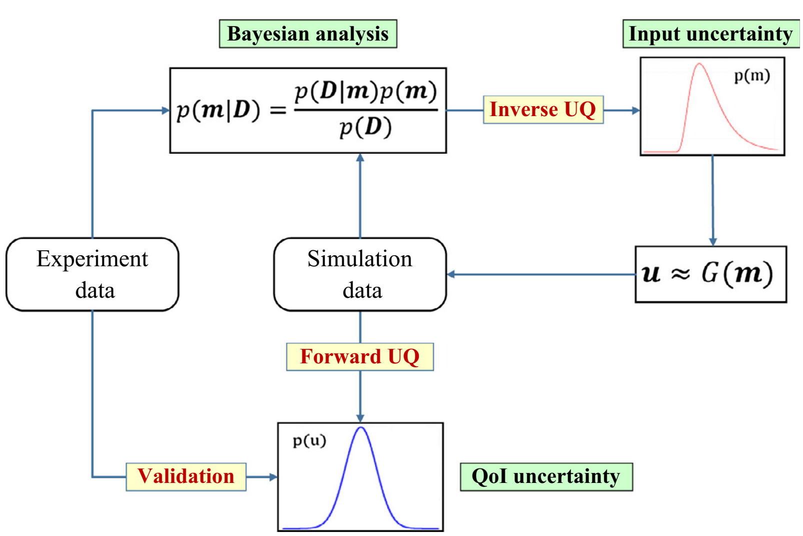

Fig. 1. UQ (forward and inverse) and validation framework.