DATA ASSIMILATION APPLIED TO PRESSURISED WATER REACTORS

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ABSTRACT

Best estimate plus uncertainty is the leading methodology to validate existing safety margins. It remains a challenge to develop and license these approaches, in part due to the high dimensionality of system codes. Uncertainty quantification is an active area of research to develop appropriate methods for propagating uncertainties, offering greater scientific reason, dimensionality reduction and minimising reliance on expert judgement. Inverse uncertainty quantification is required to infer a best estimate back on the input parameters and reduce the uncertainties, but it is challenging to capture the full covariance and sensitivity matrices. Bayesian inverse strategies remain attractive due to their predictive modelling and reduced uncertainty capabilities, leading to dramatic model improvements and validation of experiments. This paper uses state-of-the-art data assimilation techniques to obtain a best estimate of parameters critical to plant safety. Data assimilation can combine computational, benchmark and experimental measurements, propagate sparse covariance and sensitivity matrices, treat non-linear applications and accommodate discrepancies. The methodology is further demonstrated through application to hot zero power tests in a pressurised water reactor (PWR) performed using the BEAVRS benchmark with Latin hypercube sampling of reactor parameters to determine responses. WIMS 11 (dv23) and PANTHER (V.5.6.4) are used as the coupled neutronics and thermal-hydraulics codes; both are used extensively to model PWRs. Results demonstrate updated best estimate parameters and reduced uncertainties, with comparisons between posterior distributions generated using maximum entropy principle and cost functional minimisation techniques illustrated in recent conferences. Future work will improve the Bayesian inverse framework with the introduction of higher-order sensitivities.

KEYWORDS: Inverse Uncertainty Quantification, Data Assimilation, WIMS, PANTHER

1. INTRODUCTION

Despite decades of research, nuclear data contains large uncertainties that are crucial for accurate predictions of reactor analysis and beyond design basis fault studies. Predictive modelling and uncertainty quantification are an active area of research to improve results. This paper explores the use of data assimilation which has experienced a resurgence due to increased computational power and accounts for all the available experimental information and coupled simulations. It has an established history in the nuclear industry through cross-section adjustments to generate evaluated nuclear data files. Recent interest is focused on improving prediction of model outputs, measurement results, uncertainty reduction and improvements on model inputs, which often rely on speculative uncertainties with assumed probability distributions without sufficient rigour to demonstrate their appropriateness. A better estimate of the parameters and cross-parameter correlations provides a framework to challenge historic or poorly validated uncertainties, better understanding of parameters of operational importance in an ageing fleet and reduce uncertainties. Data assimilation is useful where the best estimate between the model and measurements is unclear, particularly in multi-physics problems.

The aim of this paper is to demonstrate recent data assimilation techniques applied to a Pressurised Water Reactor (PWR) when there are limited experimental observations. The problem is limited to a simple start-of-life Hot Zero Power (HZP) conditions with the inclusion of Bayesian updating on the nuclear data and also accounting for model error which is typically ignored. Section 2 discusses the background to data assimilation with sampling and sensitivity methods. The adjustments on the bank worth response parameters are shown in section 3, with new information on inter-parameter correlations followed by uncertainty reductions of nuclear data in section 3.1. WIMS 11 (dv23) and PANTHER (V.$5.6.4$) are used as the coupled reactor physics and thermal-hydraulics codes using JEFF $3.1.2$ and the 44 covariance library as a source of nuclear data uncertainties. The reactor used is Cycle 1 from the Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) [1]. The broader aim of future research is to make improved predictions of large-scale problems, demonstrate the impact of higher-order sensitivities and model adjustments with a particular interest on uncertainty reduction of model parameters.

2. DATA ASSIMILATION OVERVIEW

Data assimilation is an example of inverse uncertainty quantification and provides an intuitive derivation from multivariate probability distribution functions. Derived using Bayes' theorem, the prior function represents application information and the likelihood function provides new information, typically experimental. The product of the two is known as the posterior probability distribution function $p(x|y) \propto p(x)p(y|x)$ defined by conditional probabilities. This process can either be used individually or recursively as part of a Markov Chain where the current probability depends on the previous probability and, with increasing iteration, loses influence on the initial conditions, and is a common platform to accommodate recursive Bayesian estimation.

The key enabler in data assimilation is a weighting function between the uncertainties of the model prediction and measurements, known as the Kalman Gain matrix. It assumes all information has a degree of uncertainty and determines how measurement data influences neighbouring states. Depending on the strength of correlations, a measurement might correct the states in the neigh-

bourhood strongly or weakly. A key feature is the reduction of uncertainties as the prior positive semi-definite covariance matrix is reduced by the Kalman Gain matrix. One of the attractions of such methods is that the derivation and assumptions are clear, making it easier to interpret and challenge results with no black box approach. Problems with data assimilation include being unable to truly quantify all the prior uncertainties, poor knowledge on experimental uncertainties and variations in the sensitivities due to model error. Furthermore, the posterior distribution is an estimation approach due to the optimisation and approximations made in the prior covariance matrices.

The aim of uncertainty quantification applied to data assimilation is to improve understanding of existing models with experiment. This is known as a best estimate in both the input and output parameters. However, experiments are typically sparse relying on improvements of known measurements and using this to make predictions of unknown measurements such as rare event modelling, adjusting the input parameters or simply using the limited benchmarks available. Parameter Bayesian updating is performed using sensitivities to map inputs to outputs, and one way to perform this is to undertake a large screening exercise on a lower fidelity model to reduce the number of sensitivity calculations on higher fidelity and coupled codes. However, even this may be limited by the 'curse of dimensionality' due to the need for many code runs for both higher-order sensitivities and coupled physics simulations. Hence, adjoint sensitivity analysis or reduced-order models are pivotal for a broader range of validation and improved understanding.

The most common derivation of data assimilation algorithms is to consider Gaussian probability distributions in both the prior and likelihood functions and take the natural logarithm resulting in the cost function. For each prior there will be an associated covariance matrix which embodies all of the hypotheses about errors and uncertainties in the prior fields and is typically assumed static or time invariant. The gradient of the cost function leads to the maximum a posteriori, searching for the minimum vector of the residual $\min ||Ax^k - b||^2$, and provides an approximate solution to the linear system. A linear combination of these forms a Krylov subspace, but, given the covariance matrix is symmetric positive semi-definite, the problem is solvable using either conjugate gradients or Cholesky decomposition. A more thorough derivation uses the maximum entropy principle along with Lagrange multipliers, generating predictive results for the mean and covariances of input and output parameters, but also their correlations even when no knowledge exists about the prior correlations. The correlations between input parameters and between input and responses represent new predictive information and can also be expanded for higher-order correlations [2,3]. Other authors provide complete derivations of these formulae [2,4–6].

$$\alpha^{pred} = \alpha^0 - \left(C_{\alpha\alpha}S_{r\alpha}^{\dagger} - C_{\alpha r}\right)\left[S_{r\alpha}C_{\alpha\alpha}S_{r\alpha}^{\dagger} - S_{r\alpha}C_{\alpha r} - C_{\alpha r}^{\dagger}S_{r\alpha}^{\dagger} + C_{rr}\right]^{-1} r_d \tag{1}$$

$$C_{\alpha\alpha}^{pred} = C_{\alpha\alpha} - \left(C_{\alpha\alpha}S_{r\alpha}^{\dagger} - C_{\alpha r}\right)\left[S_{r\alpha}C_{\alpha\alpha}S_{r\alpha}^{\dagger} - S_{r\alpha}C_{\alpha r} - C_{\alpha r}^{\dagger}S_{r\alpha}^{\dagger} + C_{rr}\right]^{-1}\left(C_{\alpha\alpha}S_{r\alpha}^{\dagger} - C_{\alpha r}\right)^{\dagger} \tag{2}$$

The fundamental data assimilation algorithms are shown by Eqns. (1)–(2) for the posterior mean and covariance terms respectively. Here α represents the input parameters, r the model responses, C a covariance matrix, S a first-order sensitivity matrix and d the deviation between model and experiments. Equivalent terms exist for r^{pred}, C_{rr}^{pred} and $C_{\alpha r}^{pred}$. As shown by Eqn. (2), uncertainty reduction occurs when adding new information as a positive semi-definite matrix is subtracted from the prior quantity. This method is known as Best Estimate Results with Reduced Uncertainties

(BERRU) and represents a novel approach due to the derivation of correlations between input and output parameters and the ability to extend to higher-order contributions [2]. Similar expressions can be used with a sampled covariance approach instead of a sandwich covariance estimation. This novel approach is called Monte Carlo Bayesian (MOCABA) and has been used to include adjustment of model parameters with the use of both experiments and benchmarks [4]. Both the sampling and sensitivity methodology will be compared in this paper using WIMS 11 to perform an eigenvalue decomposition on the covariance matrix to perform direct perturbations and sampling on individual nuclides and reaction types.

2.1. Accounting for Model Error

Assigning model errors is the most challenging task in data assimilation, due to the quantity of error sources such as empirical formulation, initial and boundary conditions, poor parametrization and unresolved processes, but also the errors cannot be measured, so one can only make assumptions about them. The probability distribution and higher-order moments are almost never known and always assumed or neglected. Model error is poorly accounted for in reactor analysis and yet can often be an important source of uncertainty. It requires different expertise of different codes and is generally too costly to consider except in benchmark analysis.

A common approach in geosciences is to augment the vectors and covariance matrices as shown by Eqn. (3), where f represents the model error [7]. This is known as the weak constraint approach. It is used to adjust the prior distribution with new model information, without the need for a more rigorous cost function optimisation. It can also be used to correlate between an application and benchmark, so, if a benchmark is poorly correlated, it only has a small influence on data adjustment, as there is no additional information provided. This is the same approach taken in the MOCABA technique and is widely used to introduce other errors in data assimilation literature [4].

$$r' = \begin{pmatrix} r_0 & f_0 \end{pmatrix}, C'_0 = \begin{pmatrix} C_r & 0 \\ 0 & C_f \end{pmatrix}, C'_y = C_y, \tag{3}$$
$$S' = \begin{pmatrix} S & 0 \end{pmatrix}, r^{pred} = \begin{pmatrix} r_0^{pred} & f_0^{pred} \end{pmatrix}, C^{pred} = \begin{pmatrix} C_a^{pred} & 0 \\ 0 & C_f^{pred} \end{pmatrix}$$

This paper applies this method to the MOCABA technique such that the covariance is expressed and substituted after derivation of equations $\mathrm{diag}(C_r, C_f)$. Off-diagonal terms are used to correlate between the different cases, requiring strong understanding of the prior covariances and large sample sizes to satisfactorily determine. The WIMS-PANTHER model is compared to those generated in Monte Carlo methods [8] as a simple example.

3. HOT ZERO POWER TESTS

HZP tests provide essential measurements at the start of a reactor cycle, with useful data to compare coupled neutronics and thermal-hydraulics. 14 responses are considered, divided into rod worth, temperature coefficients and boron dilution. Sensitivity methods depend on the choice of cross-section grouping, with a group sum approach relying more strongly on averaging over energy

groups, but too many groups increases the dimension of the problem, which adds to the curse of dimensionality. In this research both were studied and results of sensitivities are calculated from finite difference for 6 nuclides and reaction types including H and O scatter, U235 fission, total nubar, U238 fission, total nubar, across 44 energy groups using covariances from the JEFF 3.1.2 data library in WIMS. First-order sensitivities are calculated, with higher-order and indirect terms to be sought in future work. For the sampling case, 60 Latin hypercube nuclear data libraries are used to construct the nuclear data covariance matrix. This is performed using a sampled data library provided in WIMS for JEFF 3.1.2. This sample size is unlikely to be sufficient for convergence of results and therefore an additional statistical error remains for future work.

Table 1: Bayesian updating on bank worth (pcm) comparing MOCABA sampling and BERRU sensitivity methods.

Case	**WIMS-PANTHER**	**Meas** $\sigma = 1.5\%$	$C_{sample}/C_{sensitive}$ **Prior**	**Sampling method Posterior**	**Sensitivity method Posterior**
D in	803 ± 11	788	0.92	789 ± 7	797 ± 4
C with D in	1254 ± 50	1203	0.67	1232 ± 13	1223 ± 5
B with D, C in	1191 ± 32	1171	0.86	1204 ± 11	1205 ± 6
A with D, C, B in	604 ± 67	548	1.21	551 ± 15	497 ± 13
SE with D, C, B, A in	511 ± 62	461	2.14	469 ± 14	477 ± 10
SD with D, C, B, A, SE in	797 ± 16	772	1.28	769 ± 6	790 ± 7
SC with D, C, B, A, SE, SD in	1128 ± 12	1099	1.05	1106 ± 5	1094 ± 4

Table 1 compares the prior and posterior results, with all measurements assimilated and assumed errors. Bank worth priors have a range of uncertainties varying from 1% to 11%. The degree of similarity between the two approaches is shown by the prior covariance ratio, with general good agreement despite only 60 Latin hypercube samples being used, and disagreements are generally minor. In all cases, the model uncertainties are reduced in both methods, with differences due to inter-parameter interactions. There is a need to improve input parameter values of which HZP provides a set of measurements for adjustment. By Bayesian updating model parameters, improved predictions can be made in regions with no experimental validation. The weak constraint method was applied to account for the model error with small adjustments to the bank worths shown in Table 2 using literature values [8]; in particular, this aids in adjusting the mean values and is cheap to estimate compared to a strong constraint approach. In practice, model error can be as significant as the nuclear data uncertainties so a broader study is required.

Figure 1 shows the posterior correlations results from the BERRU method. The covariances are normalised by the posterior standard deviations to highlight the spread of covariance. The off-diagonal terms of the parameter-parameter correlations represent new information that was unknown without data assimilation. The largest variability is seen in U235 total nubar and H scatter, and this is reflected in the parameter-response correlations in Fig. 1(b). Initial work in comparing this to sampling methods suggests good agreement despite only first-order sensitivities, although further investigation is needed for U235 total nubar bank worth correlations, H scatter, C with D in bank worth and isothermal temperature coefficients (ITC), as eigenvalue decomposition sampling

Table 2: Bayesian updating on bank worth (pcm) accounting for model error combining WIMS-PANTHER and Monte Carlo methods [8] through a weak constraint methodology.

Case	**Sampling method with model error**
D in	782 ± 6
C with D in	1234 ± 9
B with D, C in	1195 ± 8
A with D, C, B in	554 ± 6
SE with D, C, B, A in	480 ± 10
SD with D, C, B, A, SE in	781 ± 6
SC with D, C, B, A, SE, SD in	1104 ± 6

methods suggest a degree of uncertainty on these results. These techniques aid dimensional reduction studies which are pivotal in reducing the impact of the curse of dimensionality seen across uncertainty quantification methods. Future studies will increase reaction types, such as scattering and boron capture, and will focus on input parameters integrating all available measurements in Cycle 1 across burnup.

3.1. First-order uncertainty reductions on input parameters

A particular interest in data assimilation is to provide updated parameters. Nuclear data uncertainties can vary significantly on individual energy groups within a given reaction. Using a 44 covariance data library with sensitivities for each of the 6 aforementioned nuclides, the reduction between the posterior and prior parameter covariance matrices is calculated. Figure 2 highlights the percentage by which the original covariance matrix is reduced. These posterior results show modest reductions for the U238 fission and U235 total nubar cross-sections of 15–25%. Given the strong correlations with many responses, this can assist with cycle adjustments, particularly when performing predictive modelling on the broader cycle measurements. In practice, these reductions are likely to be on the smaller side, and future work will focus on how this evolves with inclusion of higher-order interactions integrated across burnup, given the limitations of first-order sensitivities.

4. CONCLUSIONS

Both the sampling and sensitivity data assimilation approaches can be used to improve understanding of uncertainties and offer a full Bayesian approach unlike other stochastic methods. Such methods may provide useful tools to cross-check expert opinion or poor agreement between experiments and simulations. The results showed similar prediction between the two approaches, despite only using 60 Latin hypercube samples. New off-diagonal parameter covariance information and parameter-response covariance information has been predicted from full core models with reduced

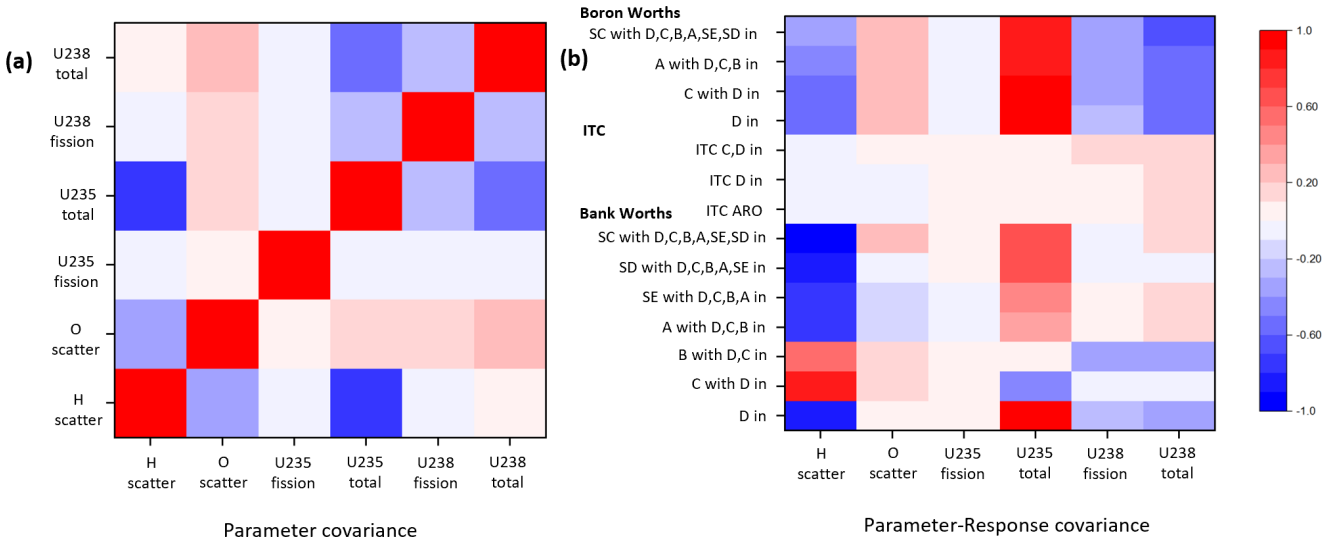

Figure 1: Input-input and input-output predicted posterior normalised covariances representing new information.

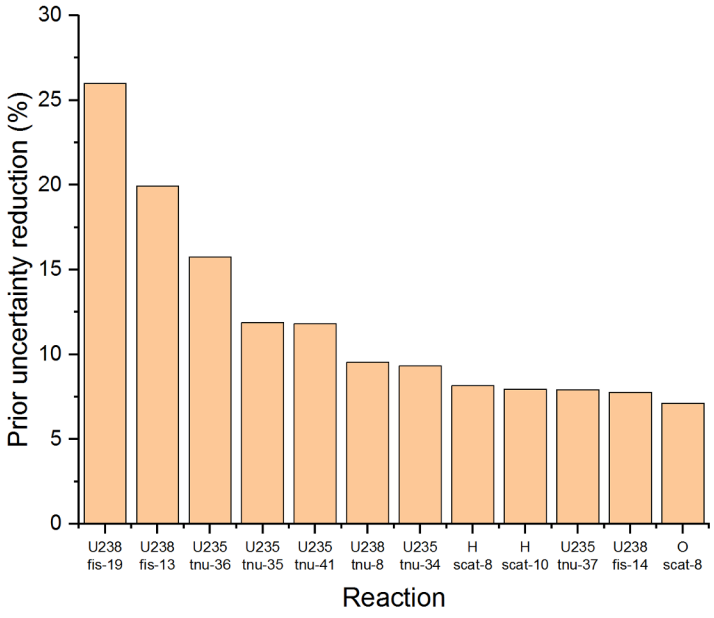

Figure 2: Percentage reduction of 44 energy group nuclear data prior uncertainty.

uncertainties. However, such techniques will benefit from high-order sensitivities or large sample sizes. Future work will focus on Cycle 1 measurements and accident scenarios which are strongly connected with irreducible uncertainties, such as the initial conditions and sparse or no available

measurements. This creates an over-reliance on priors and may not hold for different sets of initial conditions. Perhaps the largest benefits of probabilistic inference may be seen with coupled-data assimilation using coupled modelling with observations in both the thermal-hydraulic and material properties, notably at high burnup.

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