Physics-guided Covered Mapping: a new approach for quantifying experimental coverage and bias scaling

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INTRODUCTION

This summary deals with a fundamental question in any reactor model validation practice: given a body of available experiments, and an envisaged domain of reactor operating conditions (referred to as reactor application), can one develop a quantitative measure that measures the portion of the prior uncertainties of the reactor application that is covered by the available experiments? Coverage here means that the uncertainties of the reactor application are originating from and behaving in exactly the same way as those observed at the experimental conditions. This approach is valuable as it provides a scientifically defendable criterion by which experimentally measured biases can be credibly extrapolated (i.e., mapped or scaled) to biases for the reactor applications. Our proposed approach is referred to as physics-guided coverage mapping (PCM), and in this introductory summary, we will demonstrate its application to fission reactors criticality safety applications. Potential advantages of PCM over the methods of similarity (representativity), data adjustments (also known as data assimilation or model calibration) commonly employed in the nuclear community will be briefly discussed.

BACKGROUND ON MODEL VALIDATION

Model validation measures the degree to which a given reactor model is a true representation of the real reactor behavior for the intended range of reactor operation. To deem a validation exercise a success, one must be able to answer the following question with quantitative confidence: is there sufficient evidence in terms of analysis and experiments that the simulation predictions will be satisfactory for the intended reactor application? The criterion for satisfactory predictions is that the discrepancies between true and predicted future reactor responses can be bounded with high probability by pre-determined margins. And the margins are to be estimated based on a proper account of all sources of uncertainties in the simulation plus some administrative margin to account for unknown sources of uncertainties.

To perform validation, two major tasks must be accomplished. The first task is experimental in nature; it involves the construction of experiments whose design is similar to the intended reactor application, with the primary goal of measuring the discrepancies (referred to hereinafter as experimental biases) between measured and model-predicted responses. The experiments are required because no validation is credible without some level of comparison against reality. The second step is computational, wherein model predictions at reactor conditions are employed in conjunction with the experimental biases to determine the application biases and their uncertainties; the application biases estimate the expected discrepancies between the predicted and future measured responses for the reactor application. If done correctly, the estimated application biases will be close to the true application biases which are observed when the real reactor is in operation.

We will refer to this process as ‘mapping’ (sometimes referred to as ‘scaling’ or ‘extrapolation process’ by other practitioners). The mapping will describe the mathematical transformation employing experimental biases, and analysis results of the experiments and the reactor application to determine the application biases and their uncertainties.

This summary introduces a method called physics-guided coverage mapping, or in short PCM, designed to map the biases from the experimental domain to the domain of reactor application by relying solely on the physics of the simulation while taking into account all sources of simulation uncertainties. The target of the PCM methodology is the calculation of a metric referred to as ‘coverage’ which measures the portion of the prior uncertainty of the reactor application that can be explained, i.e., covered, by the experimental measurements. It is important to note that the notion of coverage or lack thereof has been employed before [1]. Our goal here is to introduce a new definition that can address some of the challenges faced by earlier definitions. For example, in the nuclear community, the term ‘similarity’ (and sometimes ‘representativity’ [2]) has been coined to quantitatively measure the resemblance between an experiment and the reactor application of interest.

To motivate the discussion we recall some of the definitions employed in the nuclear criticality community involving the use of data assimilation and similarity indices. Let the physics model describing the experiment be given by:

$$y_{\text{ex}} = f_{ex}(x,u)$$

where x are basic physics parameters (such as cross-sections) and u are the experiment’s control parameters (such as the experiment’s materials, geometry, and composition specifications, etc.). One can abstractly describe the

experimental design in terms of these control parameters, which are tuned to make sure the experiment is as similar as possible to reactor application. The y_{ex} are the responses of the experiment as predicted by the model. Let y_{ex}^{msr} be the experimental measurements corresponding to the model predictions y_{ex}. Next, define the reactor application using:

$$y_{rc} = f_{rc}(x, v)$$

where x are the same basic physics parameters employed earlier in the modeling of the experiment, and v are control parameters that describe the reactor design, e.g., size of the core, enrichment, etc. Notice that the experiments and the reactor conditions have different control parameters (i.e., u vs. v), and different functions (i.e., f_{ex} vs. f_{rc}); however, they both share x as part of their input data. Finally, the prior uncertainties for the basic physics parameters are described by a PDF $p_{pri}(x)$. To simplify the discussion, we will employ Gaussian PDFs to describe the prior parameter uncertainties. Generalization to non-Gaussian PDFs is straightforward, however it will be left to a future article. A multi-variable Gaussian distribution is fully described by a mean vector and a covariance matrix, denoted by x_{pri} and $\mathbf{C}_{pri}$, respectively.

The conventional calibration practice, depicted in Fig. 1, employs an adjustment-based approach to the calculation of reactor application biases [See Section (21) of Ref. 3]. This is done based on the assumption that the experiment biases originate from uncertainties in the basic physics parameters. A minimization search is formulated to calculate a posteriori estimate of physics parameters that minimizes the discrepancies between the measured and predicted responses. Because the number of measured responses is often much lower than the number of uncertain physics parameters, the minimization problem is expected to have an infinite number of solutions. To render a well-posed search, prior information for the physics parameters is employed to regularize (i.e., turn an ill-posed into a well-posed problem) the search, described mathematically (for the parameter Gaussian case) as follows (this approach is also referred to as Bayesian Estimation):

$$\min_{x} \left\{ \begin{array}{l} \left[y_{ex}^{msr} - f_{ex}(x,u) \right]^T \left[\mathbf{C}_{ex}^{msr} \right]^{-1} \left[y_{ex}^{msr} - f_{ex}(x,u) \right] \\ + \left[x - x_{\infty} \right]^T \left[\mathbf{C}_{pri} \right]^{-1} \left[x - x_{\infty} \right] \end{array} \right\}$$

where the first term is called the misfit term, measuring the discrepancy between measured and predicted experimental responses; the initial (i.e., prior to adjustment) value of this term is equal to the experiment bias. And the second term is called the regularization term, where x_{∞} represents the best guess for the physics parameters based on prior information, i.e., before the experimental measurements are collected. The confidence in the prior values of the parameters is described by the prior covariance matrix $\mathbf{C}_{pri}$, which is used as weight for the regularization term. This weighting ensures that parameters with very small uncertainties are hardly adjusted because they are accurately known, whereas parameters with high prior uncertainties are allowed to adjust within their prior uncertainty limits to better fit the measurements. The results of this minimization search are a set of adjusted parameter values, denoted by x_{pst}, and an updated covariance matrix, referred to as the posteriori covariance matrix, $\mathbf{C}_{pst}$.

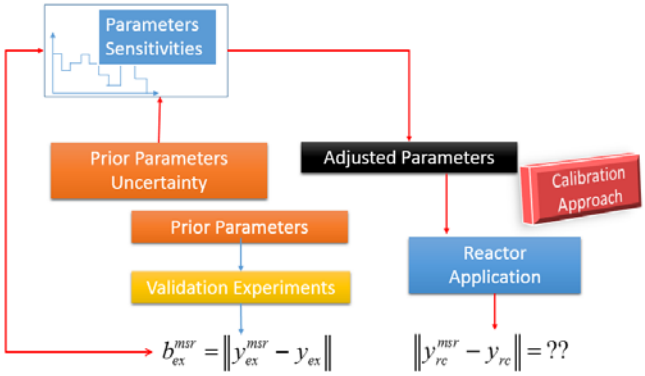


Fig 1. Adjustment-based Approach for Bias Mapping

The minimizer x_{pst} is believed to improve prior knowledge of physics parameters and is hence employed to re-evaluate the application responses as follows: let $y_{rc}^{pri} = f_{rc}(x_{pri}, v)$ and $y_{rc}^{pst} = f_{rc}(x_{pst}, v)$ represents the priori and posterior application responses, respectively. If reactor measurements are available, let them be denoted by y_{rc}^{msr}, the premise of this approach is that:

$$\left\| y_{rc}^{msr} - y_{rc}^{pri} \right\| > \left\| y_{rc}^{msr} - y_{rc}^{pst} \right\|,$$

which means that the posteriori predicted responses are closer to the measurements than the prior predictions. Using the posteriori parameter covariance matrix, the responses uncertainties calculated with the adjusted parameters can be estimated. The premise of this approach is that the posteriori responses uncertainties for the reactor application will be statistically consistent with the discrepancies between the measured and predicted future responses of the reactor application. This approach however faces several fundamental challenges, which are detailed elsewhere (see Ref [4]), but briefly summarized here. It requires adjustment of basic physics parameters, a practice that is frowned upon by physicists and practitioners, simply because there is no guarantee that the adjusted parameters will in fact improve predictions for the application. Instead, similarity indices are employed to describe in a semi-quantitative way the closeness between the experiment and the application:

$$s = \frac{g_{ex}^T \mathbf{C}_{pri} g_{rc}}{\sqrt{g_{rc}^T \mathbf{C}_{pri} g_{rc}} \sqrt{g_{ex}^T \mathbf{C}_{pri} g_{ex}}}$$

where the vectors g_{ex} and g_{rc} are the gradients of a given response, e.g., critical eigenvalue, with respect to the basic physics parameters x as calculated from the experiment and the reactor application models, respectively. This metric takes on values between zero and one to provide a single

number that measures similarity. We call it semi-quantitative because it is only used as a ball-park metric to exclude from the adjustment procedure any experiments that are not close enough to the application. Based on private communication with practitioners of similarity indices, a similarity below 0.85 is often used as the cut-off below which experiments are considered to be non-representative of the application.

The primary weakness of the data adjustment approach lies in its basic assumption - that is the observed biases are solely originating from physics parameter uncertainty. When other sources of uncertainty are prominently present, referred to as modeling uncertainty, the posteriori parameter values have to be over- or under-adjusted to account for modeling uncertainty. The impact of these over or under-adjustments may be significant enough to deteriorate the predictions for the reactor application. This is a challenging situation because it is difficult to hedge against the impact of modeling uncertainty because they are typically unknown. Over the past fifteen years, the problem of model calibration under the influence of modeling uncertainty has occupied the attention of many practitioners, including applied mathematicians and statisticians, who have made several prominent proposals to account for the impact of modeling uncertainty on the adjusted parameters [5]. This problem however is arguably far from being solved.

DESCRIPTION OF PROPOSED APPROACH

PCM overcomes the primary challenges of data adjustment techniques by attacking the problem from a different angle. Existing methods break up the problem into two steps. The first step attempts to identify the numerous sources of uncertainties, done via adjusting of the various uncertain parameters. In step two, the adjusted parameters are used to simulate the behavior of the application of interest. We attack the problem directly by asking how do the experimental and application responses relate to one another? If a relationship can be established, as discussed in Ref. [6], one can map biases and their uncertainties from the experimental domain to the application domain directly without having to identify the sources of uncertainties. Moreover, the quality of the relationship will determine the confidence by which biases can be mapped between the two domains. If many sources of uncertainties, e.g., modeling uncertainties, exist in say the application but not in the experimental domain, it will deteriorate the relationship between the two domains, and hence the mapping of biases will incur large penalty (i.e., uncertainty) due to the additional sources of uncertainties. The advantage of this approach is immediately apparent when considering that the problem of determining a relationship between the application and experimental responses is well-posed, and does not involve any inversion or optimization, thereby precluding the need for regularization.

We know describe the execution of the PCM algorithm. Assume that one is starting with *M* different experiments and a single application. Assume each experiment comes with a measured value for the response of interest, denoted as $y^{(i)}_{\text{exp},msr}$, i =1, …, *M*. Next, execute the forward models for the application and the *M* experiments and obtain the reference values for the application response y_{app} , and that of the experiments $y^{(i)}_{\text{exp}}$, i=1,2…, *M. The goal is to employ the biases* $y^{(i)}_{\text{exp}} - y^{(i)}_{\text{exp},msr}$, i=1,…, *M to determine a bias for the application response.* The PCM algorithm proceeds as follows:

1. Identify all sources of uncertainties in the experiments and the application. Let x denote the common sources, while u_i refers to the sources unique to experiment #i, and v those of the application. Examples are: x denotes cross-sections; u_i denotes the fuel to moderator ratio, geometry of the unit cell, etc., in the experiment #i, and v denotes uncertainties in one of the core parameters in the reactor application, e.g., the flow rate. Note that in general the u_i and v will be independent of one another.
2. Generate *N* samples of x, u_i, and v.
3. Execute application and *M* experiments computational models *N* times, each corresponding to one of the samples. This step represents an uncertainty analysis done for each of the experiments and the application.
4. Let the *N* responses from the application and experiment #i be denoted by vectors y and g_i both of length *N*, respectively, where i = 1,…, *M*
5. Find a relationship between the response of the application and the *M* experimental responses using the *N* training datasets. This step can be completed in many different ways. See discussion below.
6. Based on relationship in 5, determine what the application response should be, denoted by a vector y_{proj} of *N* components. This variable is expected to be different from y, because not all aspects of the application are captured by the experiments. The idea is to compare these two vectors to determine coverage.
7. Draw a scatter plot of the components of y against those of y_{proj}. If the experiments are indeed perfectly representative of the application, one would get a perfect contour that relates the two quantities. In reality, the scattered points will define a trend which describes the dependence of the application on the experiments, and the degree of the scatter will determine the uncertainty of this dependence.
8. Using measured experimental biases as input to the relationship developed in 5, determine the estimated application bias, denoted, $y_{proj,msr}$
9. Using the scatter plot in 7, determine possible values of application bias that corresponds with value of $y_{proj,msr}$

The relationship in step 5 may be determined parametrically, i.e., using response surface methods, or via a large number of non-parametric statistical techniques, e.g., order statistics, kernel density estimators, projection pursuit techniques, etc.

In this introductory presentation, we will use a simple parametric approach based on a linear surrogate model. Extension to other techniques will be part of future work. The model in Eq. 5 employed here is constructed as follows. Let the N samples for the application and experiments follow the following linear mapping:

$$y^{(i)} = \alpha_1 g_1^{(i)} + \alpha_2 g_2^{(i)} + ... + \alpha_M g_M^{(i)}, \quad i = 1, ..., N$$

This equations can be satisfied only in a least-squares sense, which is used to determine the coefficients α_i. Following that, determine q_{proj} according to step 6. The N samples of y and y_{proj} are then graphed using a scatter plot on the x and y-axes, respectively, per step 7. Per step 8, the estimated application bias is given by:

$$y_{proj,msr} = \alpha_1 \left(y^{(1)}_{\exp,msr} - y^{(1)}_{\exp} \right) + ... + \alpha_M \left(y^{(M)}_{\exp,msr} - y^{(M)}_{\exp} \right)$$

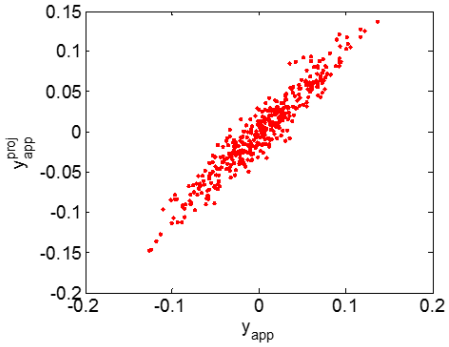
Using the scatter plot, determine the value of the application bias corresponding to estimated bias from the above equation.

NUMERICAL RESULTS

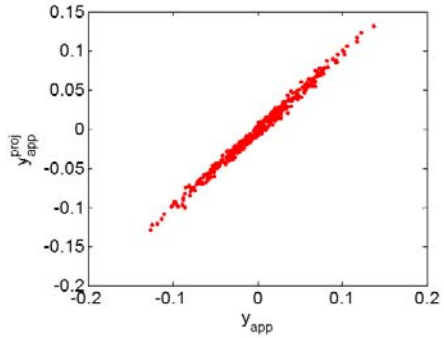
For this preliminary study, the sensitivity profiles for 31 critical experiments formed the pool of our analysis. The first K experiments (taken at K=10, and K=30) are grouped together to represent the experimental domain. Experiment #31 is taken to represent the application of interest. Using PCM, N samples for the experimental responses and the application are calculated. Based on fitting to a linear model, the application responses estimated based on the experiments are scatter-plotted against the original application responses as done in Fig. 2. This figure may be used as follow: based on the M experiments biases, calculate the application bias, and its uncertainty. Look up the calculated bias on the y-axis, and establish a band around it describing its uncertainty, and move horizontally to the scattered points, then vertically to determine the corresponding value on the x-axis, and its uncertainty. In practice, this can be done analytically using kernel density estimators, but for the sake of this introductory presentation, a graphical description is provided. The results in Fig. 2 are not surprising as they show the dependence of the application on the experiments as more experiments are added. The value of this approach is that one can see clearly the relationship between the experiments and the application, and the impact of uncertainties on the mapped biases.

CONCLUSIONS

This manuscript has introduced a data adjustment-free methodology to support the mapping of biases from the experimental to application domain, which relies on the physics of validation experiments and reactor conditions to scale experimental biases to domain of reactor operation. This is based on a joint uncertainty analysis that quantifies the dependence between the experimental and application domains; thereby providing a unique ability to map biases and their uncertainties in a credible manner, which addresses the challenges of data adjustment techniques.



(a) Coverage with 10 Experiments



(b) Coverage with 30 Experiments

Fig. 2. Application Coverage by Experiments

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