Nuclear Engineering and Technology 49 (2017) 1219–1225

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

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

Original Article

Surrogate based model calibration for pressurized water reactor physics calculations

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ARTICLE INFO

Article history:
Received 4 June 2017
Accepted 7 August 2017
Available online 19 August 2017

Keywords:
Light water reactors
Model calibration
Surrogate modeling

ABSTRACT

In this work, a scalable algorithm for model calibration in nuclear engineering applications is presented and tested. The algorithm relies on the construction of surrogate models to replace the original model within the region of interest. These surrogate models can be constructed efficiently via reduced order modeling and subspace analysis. Once constructed, these surrogate models can be used to perform computationally expensive mathematical analyses. This work proposes a surrogate based model calibration algorithm. The proposed algorithm is used to calibrate various neutronics and thermal-hydraulics parameters. The virtual environment for reactor applications-core simulator (VERA-CS) is used to simulate a three-dimensional core depletion problem. The proposed algorithm is then used to construct a reduced order model (a surrogate) which is then used in a Bayesian approach to calibrate the neutronics and thermal-hydraulics parameters. The algorithm is tested and the benefits of data assimilation and calibration are highlighted in an uncertainty quantification study and requantification after the calibration process. Results showed that the proposed algorithm could help to reduce the uncertainty in key reactor attributes based on experimental and operational data.

1. Introduction

Any mathematical model is an approximate representation of the real phenomenon of interest. Therefore, it is a common practice within engineering research communities to improve the predictability of mathematical models via model parameter calibration. Model calibration is a mathematical tool based on solving an inverse problem using the connection between experimental and operational data on one side and the mathematical model and its parameters on the other. This connection is used to improve the performance of the mathematical model by calibrating the model's parameters, along with updating their uncertainties to improve agreement of model predictions with experimental measurements and operational data.

Model calibration (sometimes referred to as data assimilation) has been used in various engineering fields, including nuclear engineering, for the enhancement of the predictions made by mathematical models and simulations [1,2]. Although very useful, model calibration analysis is hindered by two major challenges. The first is the computational burden associated with the high fidelity models (i.e., reactor core simulators). The second is the curse of dimensionality associated with the number of model parameters that will need to be calibrated (e.g., nuclear data cross-sections libraries). Both challenges are further worsened given the fact that the model calibration is an inverse optimization problem that requires multiple model executions.

Model calibration, utilizing the long operational experience with light water reactors, could improve simulation fidelity. In this work, the delayed rejection adaptive Metropolis (DRAM) algorithm [3] will be used in conjunction with reduced order modeling based surrogates, such that the end result is a practical and applicable algorithm for model calibration for large scale reactor core simulation, overcoming the two major challenges mentioned above.

DRAM is an algorithm for minimizing the samples required versus using a Markov Chain Monte Carlo algorithm. The DRAM method performs sample rejection by combining both the delayed rejection and adaptive Metropolis methods. In the delayed rejection samples are not rejected directly by the Metropolis sampler; a second stage proposal sample is generated with an acceptance probability that is calculated to guarantee convergence to the posterior probability density function. This second stage proposal depends on the previous rejected samples, yielding partial

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http://dx.doi.org/10.1016/j.net.2017.08.007

adaptation of the proposed distribution at each step of the sampling chain; therefore, the next stage can generate more reliable sample points. These refinements are local in nature and are discarded after each step [4,5]. By contrast, adaptive Metropolis relies on global adaptation of the proposed covariance based on the previously accepted samples in the chain. At certain intervals, the proposed covariance is updated to adapt information gleaned from the previous samples. This process of adaptation is introduced to improve the mixing of the chain so that it covers the target distribution more efficiently for any given number of iterations.

Reduced order modeling can facilitate the two major challenges mentioned earlier (high computational cost and the curse of dimensionality). Mathematical surrogates can address the first problem (the computational burden associated with running the high fidelity reactor core simulators). By contrast, reducing the dimensionality of the parameters of interest by identifying the influential degrees of freedom (DoFs) using the algorithms presented in Chapter 2 and Chapter 3 of Ref. [6] will address the second problem (the curse of dimensionality).

Ref. [1] introduced high order predictive model calibration algorithms and applied them to relatively large scale applications, while Ref. [2] performed model calibration for a few thermal-hydraulic parameters using a lower order surrogate to replace the actual thermal-hydraulics simulator. This work will employ polynomial surrogate models to substitute for the original coupled models in the virtual environment for reactor applications-core simulator (VERA-CS), which uses MPACT (Michigan Parallel Characteristics Transport Code) as a neutronics model, COBRA-TF (COolant-Boiling in Rod Arrays-Two Fluids) as a sub-channel thermal-hydraulics model, and ORIGEN (The Oak Ridge Isotope Generation) for the depletion of the fuel [7]. Therefore, this work performs model calibration for a three-dimensional core depletion problem with thermal-hydraulics feedback. Finally, cross-sections (high dimensional parameter) will be calibrated along with the few thermal-hydraulics parameters considered here. Verification is completed using synthetic data, that is, data generated using VERA-CS with perturbed parameters, to determine if the actual parameter perturbations can be assessed and ultimately used to enhance the uncertainty associated with the responses of interest [5].

2. Surrogate based data assimilation and model calibration

Referring to Ref. [3], it can be noted that several steps make DRAM limited to small-to-medium parameter dimensionality problems with reasonable computational burden. If the model is complex and characterized with high computational cost, then DRAM is no longer a practical algorithm. Therefore, in this section, a subspace-based surrogate model with a smaller number of DoFs will be used to replace the original model of interest, VERA-CS. Ref. [6] proposes gradient-based and gradient-free algorithms for identifying the important and influential DoFs for single and multi-physics modeling. Since the gradient calculation capability is not always available, the gradient-free approach will be used in this work to identify the influential DoFs in the form of basis vectors.

Once, the basis is determined (**U**), a second order goal-oriented surrogate will be constructed as follows:

$$f \approx \tilde{f} = \bar{S}_1^T \Delta\bar{x} + \left(\bar{S}_2^T \Delta\bar{x}\right)^2$$

where f is the response of interest (e.g., multiplication factor, maximum fuel pin power, and maximum fuel pin temperature), and $\Delta\bar{x}$ is the variation in the parameters of interest from the reference values (e.g., cross-sections, fuel pellet-clad gap conductivity, and grid loss coefficient).

In order to reduce the number of model runs required to construct the surrogate form, the gradient-free approach mentioned before is used to calculate the basis matrix (**U**) of the lower dimensional subspace approximation for the parameters' space. The columns of matrix **U** represent the influential DoFs. Before discussing how the matrix **U** is used in constructing the surrogate, it is worth mentioning that once the influential DoFs are determined, the remaining DoFs are actually ignored, which obviously introduces a source of error in the algorithm. Fortunately, the error introduced by this truncation process can be quantified and upper bounded using the theory presented in Ref. [8] and used in [2,6]. To summarize this error upper bound equation, let us assume that vector $\bar{y}$ (represents some physical quantity) is assumed to vary along the DoFs or basis represented by the columns of matrix $\mathbf{U_F}$; then if only the influential DoFs are identified and collected in matrix **U** (which is a sub matrix of the full matrix $\mathbf{U_F}$) then the error in representing the variations in the physical quantity $\bar{y}$ via **U** can be upper bounded via the following expression:

$$\varepsilon_{upper} = 10\sqrt{\frac{2}{\pi}}\max_{j=1,\ldots p}\left\|\left(\mathbf{I}-\mathbf{U}\mathbf{U}^T\right)\bar{y}_j\right\|_2$$

This upper bound (ε_{upper}) is guaranteed with a success probability of $1-10^{-p}$ [8] where p is the number of extra snapshots used to compute that upper bound. For more information about the theory behind this error upper bund estimation and its applications, refer to [6,8].

The goal of the surrogate here is to employ it to perform model calibration analysis, so that the uncertainty and mean of each parameter might be updated. The implication is that the parameter perturbations ($\Delta\bar{x}$) generated to determine the influential DoFs and surrogate model are random within the interval of interest. This contrasts with an uncertainty quantification application, where parameter perturbations would be based upon sampling the parameters' probability distribution functions.

An efficient goal-oriented surrogate can be constructed as follows:

$$f \approx \tilde{f} = \overbrace{\bar{\beta}_1^T\mathbf{U}}^{\bar{\beta}_{1,r}^T}\ \overbrace{\mathbf{U}^T\Delta\bar{x}_{rand}}^{\Delta\bar{\alpha}} + \left(\overbrace{\bar{\beta}_2^T\mathbf{U}}^{\bar{\beta}_{2,r}^T}\ \overbrace{\mathbf{U}^T\Delta\bar{x}_{rand}}^{\Delta\bar{\alpha}}\right)^2$$
$$= \bar{\beta}_{1,r}^T\Delta\bar{\alpha} + \left(\bar{\beta}_{2,r}^T\Delta\bar{\alpha}\right)^2 \quad (1)$$

where $\Delta\bar{x}_{rand}$ is an input vector generated by randomly sampling the parameters. Given that $\mathbf{U}\in\mathbb{R}^{n\times r}$ and $\Delta\bar{\alpha} = \mathbf{U}^T\Delta\bar{x}_{rand}\in\mathbb{R}^r$, $\bar{\beta}_{1,r}^T = \bar{\beta}_1^T\mathbf{U}\in\mathbb{R}^r$ and $\bar{\beta}_{2,r}^T = \bar{\beta}_2^T\mathbf{U}\in\mathbb{R}^r$, in order to determine the unknown elements of $\bar{\beta}_{1,r}$ and $\bar{\beta}_{2,r}$ the model needs to be run $2r$ times so that the coefficients are determined (where r is the number of influential DoFs or the rank of matrix **U** which is the dimension of the identified subspace).

The surrogate based algorithm proposed here depends on two main points: first, identifying the important DoFs via methods of subspace analysis (refer to Chapter 3 in [6]). Second, once the important DoFs are determined in the form of the basis of a subspace, these bases can be used to form surrogate models $\tilde{f}$ (e.g., polynomial or Gaussian process) which can replace the original computationally expensive model f. The following is a summary of the algorithm for Surrogate Based Model Calibration (SBMC): (1) Construct the basis of the lower dimensional subspace approximation of the parameter space (**U**); (2) construct the goal-