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An efficient Bayesian uncertainty quantification approach with application to k-ω-γ transition modeling

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ABSTRACT

An efficient Bayesian uncertainty quantification approach is proposed, which combines the adaptive high dimensional model representation technique (HDMR) and stochastic collocation (SC) method based generalized polynomial chaos (gPC) to construct the surrogate for sampling procedure in Bayesian calibration step. Specifically, the adaptive HDMR technique is used to decompose the original high dimensional problems into several lower-dimensional subproblems, which are subsequently solved with the gPC-based SC method. Then the Bayesian calibration and prediction are carried out with the so-constructed surrogate model. A new indicator based on the variance of the corresponding component function is employed to identify the important components of the HDMR, instead of the original one based on the impact on the output mean, as the input parameters that can be well informed in the inverse problem are the ones that the model output is sensitive to. Further, a rigorous convergence study of the approximate posterior to the true posterior is carried out for the proposed approach. Its applications to both a simple mathematical function and a complex fluid dynamic model, i.e. k-ω-γ transition model, are investigated, demonstrating both its efficiency and accuracy. In the application to k-ω-γ transition model, the results show not only a quantified uncertainty overlapping well with the experimental data, but also a great improvement of the match between the prediction mean and the experimental data, which may be due to the further account of the intermittency through the spread of the model parameters.

1. Introduction

Hypersonic boundary layer transition is not only of fundamental interest in fluid dynamics, it is also of great practical relevance in the design of many aerodynamic configurations at hypersonic speeds. Despite the rapid development of Direct numerical simulation (DNS) technique, Reynolds-averaged-Navier-Stokes (RANS) model and empirical e^N method are still the main tools for transition predictions in engineering applications, due to its affordability compared to DNS. A local-variable-based RANS model, namely k-ω-γ model, has been proposed recently, which can successfully simulate three-dimensional (3-D) high-speed aerodynamic flow transition with a reasonably wide range of Mach numbers [1,2]. However, flow transition to turbulence is a very complex process, involving receptivity process, linear modal growth, mode interaction, final breakdown to turbulence etc. [3], which cannot be correctly simulated by RANS model. Transition prediction with RANS model is highly unreliable and the aim of this work is to quantify the uncertainty of the quantity of interest (QoI) in the hypersonic boundary layer transition simulations with k-ω-γ model.

In the pioneering work of Kennedy and O'Hagan [4], the Bayesian calibration technique for a general computer model is presented and the uncertainties are classified into parameter uncertainty, model inadequacy, residual variability, parametric uncertainty, observation error and code uncertainty. The uncertainty of RANS predictions mainly comes from the first two sources, parameter uncertainty and model inadequacy. The former represents the uncertainty due to the lack of knowledge of the model parameters and the latter represents the discrepancy between true physical observation and model output at optimal model parameters. A number of studies have focused on the parameter uncertainty. Cheung et al. [5] have applied Bayesian uncertainty analysis to Spalart-Allmaras (SA) turbulence model for wall-bounded incompressible turbulent flow at variable pressure gradients. They employed three different stochastic models for inadequacy terms and compared them in terms of model plausibility and prediction of QoIs. Oliver and Moser [6] extended the work of Cheung et al. by considering four stochastic extensions of four eddy viscosity turbulence models. They proposed a more complex stochastic model to take account of the multi-scale structure of the boundary layer. In

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Ref. [7], Edeling et al. estimated the parameter variability within and across the scenarios (i.e. at different pressure gradients) under the Bayesian framework. Further, they [8] utilized Bayesian Model-Scenario Averaging approach to synthesize the results of 5 turbulence models at 14 scenarios, resulting a substantial improvement in both prediction mean and variance. Bayesian parameter estimation was also used for other flow configurations, e.g. Jet-in-Crossflow [9] etc. Besides, parameter uncertainty of RANS models has also been assessed in Ref. [10], with the input uncertainty imposed through a prior distribution, based on an extensive literature survey about the parameter dispersion.

Besides parameter uncertainty mentioned above, model-inadequacy is also a major source of uncertainty in RANS prediction and quantifying and reducing this uncertainty have raised the research interests recently in the field. Dow and Wang [11] employed the Bayesian approach to infer the turbulent viscosity from DNS data. In Ref. [12], Emory et al. proposed an approach to quantify the uncertainty directly through Reynolds stress. In Ref [13], Gorle and Iaccarino carried out uncertainty quantification of turbulent scalar flux models, taking account of the uncertainty directly through Reynolds stress. In Ref. [14], Duraisamy et al. proposed a data-driven approach for turbulence and transition modeling, which consists mainly of injecting the functional form of deficiencies inferred by experimental data into simulations to obtain more accurate predictions. A data-driven, physics-informed Bayesian approach has been proposed recently by Xiao et al. [15], taking account of the model-form uncertainty directly through Reynolds stress and an iterative ensemble Kalman method was used to incorporate the prior knowledge and the experimental data.

The RANS turbulence models have been the main focus of the previously mentioned work. The research of uncertainty quantification for RANS transition modeling is rather limited. An exception is the work of Pecnik et al. [16], in which they applied UQ for laminar-turbulent transition in turbo-machinery configurations, using the $\gamma - \tilde{R}e_{\theta t}$ model of Menter et al. [17], but only a forward uncertainty propagation is carried out and the input uncertainty is imposed through a prior distribution. Bayesian uncertainty analysis provides a rigorous approach to quantify the uncertainty arising from the mathematical modeling and simulation, and to incorporate the prior knowledge and experimental data systematically, through Bayesian data updating. Thus in this work, we apply the Bayesian framework to quantify the uncertainty arising from the k-ω-γ transition model in hypersonic transition simulations. We focus on the parameter uncertainty and the model inadequacy is simply termed as a multiplicative Gaussian random variable, as in the work [5]. Modeling the inadequacy terms requires more physical insight of transition process and is a RANS modeling issue rather than a UQ of an existed model. In this work we restrict ourselves to the latter issue and treat k-ω-γ model as a black box.

A key step in this framework is the Bayesian calibration. After identifying the prior distribution of the input parameters and constructing the stochastic model, the posterior distributions of the model parameters are obtained through Bayes' rule. This procedure usually requires a sampling method, e.g. Markov chain Monte-Carlo (MCMC) [18]. A large number of model evaluations, typically tens of thousands, are required in the sampling procedure, which are computationally expensive. A number of methods exist in the literature to reduce the computational cost while retaining the non-intrusiveness of the corresponding approach, e.g. [19,20]. In Ref. [21], Ma and Zabaras proposed an adaptive version of high dimensional model representation technique (HDMR) to decompose the original high dimension problem into lower dimension subproblems and solved them with the adaptive sparse grid collocation (ASGC) method [22] they proposed previously. The efficiency of this approach is demonstrated with some mathematical functions and also with a set of fluid-mechanic problems. In Ref. [23] Edeling et al. improved the original Simplex-stochastic collocation (SSC) [20] method and also combined it with the adaptive HDMR technique, resulting in an improved scalability. They applied this approach in a nozzle and an airfoil flow. These approaches have only been applied in the forward problem and their application to inverse problems hasn't been explored yet. Marzouk and Xiu [24] proposed a stochastic collocation approach to Bayesian inference in inverse problems and conducted a rigorous error analysis for the approximate posterior. Several examples were carried out to demonstrate the efficiency of the proposed method, including a Burgers' equation case and a genetic toggle switch case in biology.

In this paper we combine the adaptive high-dimensional stochastic model representation (HDMR) technique [21] with the stochastic collocation (SC) approach based on generalized polynomial chaos (gPC) [24], to construct the surrogate model. Then this surrogate model is used for Bayesian inference in the inverse problem. This idea is inspired by the work of Ma and Zabaras [21], in which they combined the HDMR technique with the adaptive sparse grid collocation (ASGC) [22] method to solve the forward problem. The proposed approach can be seen as an extension of the stochastic collocation approach proposed by Marzouk and Xiu [24], by integrating it into the high dimensional model representation framework.

The paper is organized as follows: the Bayesian uncertainty quantification framework is described in Section 2. In Section 3 the surrogate model construction approach is described, including the gPC-based stochastic collocation method and the HDMR technique. The algorithm is summarized in Section 4. In Section 5 we demonstrate the accuracy and efficiency of the proposed method through a simple mathematical function. A comparison between the proposed method and the exact model is given. After testing our approach with this simple mathematical function, we apply the approach to k-ω-γ transition modeling in hypersonic transition simulations in Section 6. The results are given in Section 6.4, including both the posterior distribution of the input parameters and the prediction mean with quantified uncertainty. Finally the conclusion is drawn in Section 7.

2. Bayesian uncertainty quantification framework

2.1. General review

This part provides a brief description of the UQ framework, following the work of [5,7]. The main steps are the specification of the flow class and quantity of interest (QoI), the collection of experimental data, the construction of the stochastic model, the Bayesian calibration, and validation and prediction. As is pointed out in Ref. [5], whether a model is considered valid or not depends on its ability to predict the QoIs to the required accuracy and precision, rather than to predict all aspects of the physical world. Thus the identification of the QoIs is a key issue and should be kept in mind during the whole uncertainty quantification process. In this work, we assume the QoIs are observable for the corresponding experiments and thus we use the observation of QoIs as the data to inform the model parameters.

In Bayesian framework, various forms of uncertainty, whether aleatoric or epistemic, are all represented through probability. Thus we can characterize the input parameter uncertainty by their probability density function (PDF). In the Bayesian calibration step, the posterior distributions of the parameters are obtained through Bayes' rule:

$$p(\mathbf{z}|\mathbf{d}) = \frac{p(\mathbf{d}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{d})} \tag{1}$$