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BAYESIAN UNCERTAINTY QUANTIFICATION AND PROPAGATION USING ADJOINT TECHNIQUES

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The Bayesian inference framework for quantifying and propagating uncertainties in computational models of engineering systems has been adequately developed and widely used. The framework aims at the selection among alternative plausible model structures to represent physical phenomenon and the unmodelled dynamics, estimation of the uncertainties in the parameters of these model structures, as well as propagation of uncertainties through the model to make robust predictions of output quantities of interest (QoI), consistent with available experimental measurements.

The Bayesian tools for identifying system and uncertainty models as well as performing robust prediction analyses are Laplace methods of asymptotic approximation and stochastic simulation algorithms [1]. In analytical approximation, a Gaussian distribution is used to approximate the posterior distribution of the uncertain parameters. The most probable value of the parameters is obtained by minimizing the function defined as the minus of the logarithm of the posterior distribution and the covariance matrix of this posterior distribution is defined using asymptotic expansion as the inverse of the Hessian matrix of the aforementioned function, which is expressed as the deviation of the computed quantities from corrensponding experimental measurements. The Laplace asymptotic approximation is also used to propagate the computed uncertainties of the model parameters to compute the uncertainty in output QoI. The analytical approximations of the multi-dimensional probability integrals that arise in the propagation of uncertainties involve evaluations of appropriate objective function derivatives and Hessians. Theoretical and computational issues involved in solving the optimization problems and computing the Hessian matrices are integrated in the Bayesian framework by developing direct differentiation and higher-order adjoint formulations. Analytical techniques have computational advantages since they require a moderate number of system re-analyses in comparison to the very large number of system re-analyses needed in the stochastic simulation algorithms. This computational efficiency, however, comes with the extra burden of developing the adjoint formulations and integrating them in system simulation software, a procedure that can be quite cumbersome for a number of computational models employed in engineering simulations.

Theoretical and computational developments are demonstrated by applying the proposed framework on computational solid mechanics and fluid dynamics problems. In particular, in computational fluid dynamics applications the proposed framework is applied for the estimation of the parameters of the Spalart-Allmaras turbulence model based on velocity and Reynolds stress measurements at a backward facing step flow. Two models are considered for the correlation of the computational errors. The first one is based on a spatial correlation length model where the computational errors are assumed correlated according to their spatial distance and the second one disregards any spatial correlation. Results clearly demonstrate that the measurements provide information for estimating three to five among the eight parameters of the turbulence model, while the rest of the parameters are insensitive to the information contained in the data. Model validation using the experimental measurements suggest that the Spalart-Allmaras model is not adequate enough to accurately predict velocities and Reynolds stresses in certain region in the flow domain where flow separation phenomena are dominant. This is manifested by the high prediction error uncertainty in these regions in relation to the prediction uncertainty arising from the turbulence model parameter uncertainty. Among the two prediction error model classes considered, the spatially correlated one is clearly promoted as the best model by the Bayesian model selection methodology, confirming recent results stating the importance of including spatial correlation in prediction error models.

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