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Bayesian Model Calibration with Interpolating Polynomials based on Adaptively Weighted Leja Nodes

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Abstract. An efficient algorithm is proposed for Bayesian model calibration, which is commonly used to estimate the model parameters of non-linear, computationally expensive models using measurement data. The approach is based on Bayesian statistics: using a prior distribution and a likelihood, the posterior distribution is obtained through application of Bayes' law. Our novel algorithm to accurately determine this posterior requires significantly fewer discrete model evaluations than traditional Monte Carlo methods. The key idea is to replace the expensive model by an interpolating surrogate model and to construct the interpolating nodal set maximizing the accuracy of the posterior. To determine such a nodal set an extension to weighted Leja nodes is introduced, based on a new weighting function. We prove that the convergence of the posterior has the same rate as the convergence of the model. If the convergence of the posterior is measured in the Kullback–Leibler divergence, the rate doubles. The algorithm and its theoretical properties are verified in three different test cases: analytical cases that confirm the correctness of the theoretical findings, Burgers' equation to show its applicability in implicit problems, and finally the calibration of the closure parameters of a turbulence model to show the effectiveness for computationally expensive problems.

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1 Introduction

Estimating model parameters from measurements is a problem of frequent occurrence in many fields of engineering and many different approaches exist to solve this prob-

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lem. We consider non-linear calibration problems (or inverse problems) where a forward evaluation of the model is computationally expensive. The approach we follow is of a stochastic nature: the unknown parameters are modeled using probability distributions and information about these parameters is inferred using Bayesian statistics. This approach is often called *Bayesian model calibration*.

Bayesian model calibration [19, 32, 33] is a systematic way to calibrate the parameters of a computational model. By means of a statistical model to describe the relation between the model and the data, the calibrated parameters are obtained in the form of a random variable (called the *posterior*) by means of Bayes' law. These random variables can then be used to assess the uncertainty in the model and to make future predictions. This procedure is well-known in the field of Bayesian statistics, where the goal is to infer unmeasured quantities from data. The calibration approach has already been applied many times, for example to calibrate the closure parameters of turbulence models [7, 11]. A similar example is considered in this work.

Possibly the largest drawback of Bayesian model calibration is the expensive sampling procedure that is necessary. Because the posterior depends to a large extent on the model, which is only known implicitly (e.g. a computer code numerically solving a partial differential equation), determining a sample from the posterior is mostly done using Markov chain Monte Carlo (MCMC) methods [14, 25], requiring many expensive model evaluations. Improvements have been made to accelerate these MCMC methods, e.g. the DREAM algorithm [39] or adaptive sampling [42]. Replacing the sampling procedure itself is also possible, e.g. methods based on sparse grids [6, 22] or Approximate Bayesian Computation [2, 9, 20]. However, this encompasses stringent assumptions on the statistical model or still requires many model runs as the shape of the posterior is unknown.

A different approach is followed in the current article. In essence we are following the approach of Marzouk et al. [24], which has been used several times in literature [1, 4, 23, 28, 31, 44–46]. The key idea in our procedure is to replace the model in the calibration step with a *surrogate* (or *response surface*) that approximates the computationally expensive model. MCMC can then be used to sample the resulting posterior without a large computational overhead.

Various approaches to construct this surrogate in a Bayesian context exist, for example Gaussian process emulators [36] or non-intrusive polynomial approximations [43]. In this work the latter is considered, because polynomial approximations provide high order (up to exponential) convergence for sufficiently smooth functions. Contrary to the commonly used pseudo-spectral projection methods, which are commonly known as generalized Polynomial Chaos Expansions, we choose to use interpolation of the computationally expensive model. The reason for this is that the error of a polynomial interpolant is usually measured using the absolute error (the L^∞ norm), contrary to the mean squared error (the L^2 norm) that is used for the pseudo-spectral approaches. As the model is used as input in the Bayesian analysis, having absolute error bounds on the surrogate significantly simplifies the analysis. Moreover, the convergence of a pseudo-spectral expansion deteriorates significantly if the surrogate is not constructed using the statistical model [21]. This