

Chapter 3

Fast Computing Techniques for Bayesian Uncertainty Quantification in Structural Dynamics

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Abstract A Bayesian probabilistic framework for uncertainty quantification and propagation in structural dynamics is reviewed. Fast computing techniques are integrated with the Bayesian framework to efficiently handle large-order models of hundreds of thousands or millions degrees of freedom and localized nonlinear actions activated during system operation. Fast and accurate component mode synthesis (CMS) techniques are proposed, consistent with the finite element (FE) model parameterization, to achieve drastic reductions in computational effort when performing a system analysis. Additional substantial computational savings are also obtained by adopting surrogate models to drastically reduce the number of full system re-analyses and parallel computing algorithms to efficiently distribute the computations in available multi-core CPUs. The computational efficiency of the proposed approach is demonstrated by updating a high-fidelity finite element model of a bridge involving hundreds of thousands of degrees of freedom.

Keywords Bayesian inference • Structural dynamics • Component mode synthesis • Surrogate models • HPC

3.1 Introduction

In structural dynamics, Bayesian inference [1–3] is used for quantifying and calibrating uncertainty models based on vibration measurements, as well as propagating these modeling uncertainties in system simulations to obtain updated robust predictions of system performance, reliability and safety [4]. The Bayesian tools for identifying system and uncertainty models as well as performing robust prediction analyses are Laplace methods of asymptotic approximation and more accurate stochastic simulation algorithms, such as MCMC [5] and Transitional MCMC [6]. These tools involve solving optimization problems, generating samples for tracing and then populating the important uncertainty region in the parameter space, as well as evaluating integrals over high-dimensional spaces of the uncertain model parameters. A moderate to very large number of repeated system analyses are required to be performed over the space of uncertain parameters. Consequently, the computational demands depend highly on the number of system analyses and the time required for performing a system analysis.

To reliably update models, high fidelity FE model classes, often involving a large number of DOFs, should be introduced to simulate structural behavior. For such large-order finite element models the computational demands in implementing asymptotic approximations as well as stochastic simulation techniques may be excessive. The present work proposes methods for drastically reducing the computational demands at the system, algorithm and computer hardware levels involved in the implementation of Bayesian tools. At the system level, CMS techniques [7] are integrated with Bayesian techniques to efficiently handle large-order models of hundreds of thousands or millions degrees of freedom and localized nonlinear actions activated during system operation. Fast and accurate CMS techniques are obtained [8], consistent with the FE model parameterization, to achieve drastic reductions in computational effort. The CMS allows the repeated computations to be carried out in a significantly reduced space of generalized coordinates. At the level of the TCMC algorithm, surrogate models are adopted to drastically reduce the number of computationally expensive full model runs. At the computer hardware level, parallel computing algorithms are used to efficiently distribute the computations in available multi-core CPUs [9].

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3.2 Bayesian Uncertainty Quantification and Propagation Framework

Consider a class M_m of structural dynamics models used to predict various output quantities of interest $f(\underline{\theta}_m|M_m)$ of a system, where $\underline{\theta}_m$ is a set of parameters in this model class that need to be estimated using experimental data $D \equiv \{\hat{y}\}$. Following a Bayesian formulation [2, 3] and assuming that the observation data and the model predictions satisfy the prediction error equation

$$\hat{y} = f(\underline{\theta}_m|M_m) + \underline{e} \quad (3.1)$$

where the error term $\underline{e} \sim N(\underline{0}, \Sigma)$ is a zero-mean Gaussian vector with covariance $\Sigma \equiv \Sigma(\underline{\theta}_e)$ depending on the parameters $\underline{\theta}_e$ of the prediction error model class M_e , the updated distribution $p(\underline{\theta}|D, M)$ of the augmented parameter set $\underline{\theta} = (\underline{\theta}_m, \underline{\theta}_e)$, given the data D and the combined model class $M = (M_m, M_e)$, results from the application of the Bayes theorem as follows

$$p(\underline{\theta}|D, M) = \frac{p(D|\underline{\theta}, M)\pi(\underline{\theta}|M)}{p(D|M)} \quad (3.2)$$

where

$$p(D|\underline{\theta}, M) = \frac{|\Sigma(\underline{\theta}_e)|^{-1/2}}{(2\pi)^{N/2}} \exp\left[-\frac{1}{2}J(\underline{\theta}; M)\right] \quad (3.3)$$

is the likelihood of observing the data from the model class,

$$J(\underline{\theta}; M) = [\hat{y} - f(\underline{\theta}_m|M)]^T \Sigma^{-1}(\underline{\theta}_e) [\hat{y} - f(\underline{\theta}_m|M)] \quad (3.4)$$

is the measure of fit between the experimental and model predicted properties, $\pi(\underline{\theta})$ is the prior probability distribution of the model parameters based on previous knowledge and/or user experience, and $p(D|M)$ is the evidence of the model class.

The Bayesian probabilistic framework can also be used to compare two or more competing model classes and select the optimal model class based on the available data. Consider a family M_i , $i = 1, \dots, \kappa$, of κ alternative, competing, parameterized FE and prediction error model classes, and let $\underline{\theta}_i \in R^{N_{\theta_i}}$ be the free parameters of the model class M_i . The posterior probabilities $P(M_i|D)$ of the various model classes given the data D is [10, 11]

$$P(M_i|D) = \frac{p(D|M_i)P(M_i)}{p(D|M_1, \dots, M_\kappa)} \quad (3.5)$$

where $P(M_i)$ is the prior probability and $p(D|M_i)$ is the evidence of the model class M_i . The optimal model class M_{best} is selected as the one that maximizes $P(M_i|D)$ given by (3.5).

For large enough number of measured data, the posterior distribution of the model parameters in (3.2) can be asymptotically approximated by a Gaussian distribution [3] centered at the most probable value $\hat{\theta}$ of the model parameters with covariance equal to the inverse of the Hessian $h(\theta)$ of the function

$$g(\theta; M) = -\ln p(D|\underline{\theta}, M) = \frac{1}{2}J(\underline{\theta}_m; M) + \frac{1}{2}|\Sigma(\underline{\theta}_e)| - \ln \pi(\underline{\theta}|M) \quad (3.6)$$

evaluated at the most probable value $\hat{\theta}$ of the model parameters. The most probable value $\hat{\theta}$ maximizes the posterior probability distribution $p(\underline{\theta}|D, M)$ or, equivalently, minimizes the function $g(\underline{\theta}; M)$. For model selection, an asymptotic approximation based on Laplace's method is also used to give an estimate of the integral involved in the estimation of the evidence $p(D|M)$ in (3.2) and (3.5) [11]. For the case for which analytical expressions for the gradient of $J(\underline{\theta}; M)$ with respect to the structural model parameters θ_m are available, computationally efficient gradient-based optimization algorithms can be used to obtain the optimal value of the model parameters by minimizing the function $g(\underline{\theta}; M)$. Specifically, for linear structural dynamics models and experimental data consisting of modal frequencies and mode shapes, such analytical expressions are available and can be computed using efficient adjoint techniques (e.g. [12]). However, there are certain classes of nonlinear systems where such analytical expressions or adjoint techniques are not applicable or it is inconvenient to introduce within commercially available structural dynamics solvers. In such cases, non-gradient-based optimization algorithms can be used to obtain the most probable value of the model parameters. Once the most probable value has been computed, the Hessian required in the asymptotic approximation can be estimated using either higher-order adjoint techniques [12], if applicable, or using numerical differentiation techniques.

It should be noted that the asymptotic expression is approximate. Moreover, even for large number of experimental data, it may fail to give a good representation of the posterior probability distribution in the case of multimodal distributions. In addition, the asymptotic approximation fails to provide acceptable estimates for un-identifiable cases manifested for relatively large number of model parameters in relation to the information contained in the data. For more accurate estimates, one should use stochastic simulation algorithms (e.g. MCMC [5], Transitional MCMC – TMCMC [6], Delayed Rejection Adaptive Metropolis – DRAM [13]) to generate samples that populate the posterior probability distribution function in (3.2) and then evaluate the integrals involved in propagating uncertainties into robust predictions. Among the stochastic simulation algorithms available, the transitional MCMC algorithm [6] is one of the most promising algorithms for selecting the most probable model as well as finding and populating with samples the importance region of interest of the posterior probability distribution, even in the unidentifiable cases and multi-modal posterior distributions. In addition, the TMCMC method yields an estimate of the evidence $p(D|M)$ of a model class M , required for model class selection [10, 14], based on the samples generated by the algorithm.

The samples generated at the final stage of the TMCMC algorithm can further be used for estimating the probability integrals encountered when interested in robust predictions of various performance quantities of interest. Specifically, consider an output quantity q of interest in structural dynamics simulations. Posterior robust predictions of q are obtained by taking into account the updated uncertainties in the model parameters given the measurements D . Let $p(q|\underline{\theta}, M)$ be the conditional probability distribution of q given the values of the parameters. Using the total probability theorem, the posterior robust probability distribution $p(q|D, M)$ of q , taking into account the model M and the data D , is given by Papadimitriou et al. [4]

$$p(q|D, M) = \int p(q|\underline{\theta}, M)p(\underline{\theta}|D, M)d\underline{\theta} \quad (3.7)$$

as an average of the conditional probability distribution $p(q|\underline{\theta}, M)$ weighting by the posterior probability distribution $p(\underline{\theta}|D, M)$ of the model parameters. Let also $G(q)$ be a function of the output quantity of interest q . A posterior robust performance measure of the system given the data D is

$$E[G(q)|D, M] = \int G(q)p(\underline{\theta}|D, M)d\underline{\theta} \quad (3.8)$$

The evaluation of the multi-dimensional integrals in (3.7) and (3.8) cannot be performed analytically. Asymptotic approximations are given in [4]. Alternatively, stochastic simulation methods can be conveniently used to estimate the integral from the samples $\underline{\theta}^{(i)}$, $i = 1, \dots, N$, generated from the posterior probability distribution $p(\underline{\theta}|D, M)$. In this case, the integrals (3.7) and (3.8) can be approximated by

$$f(q|D, M) \approx \frac{1}{N} \sum_{i=1}^N f(q|\underline{\theta}^{(i)}, M) \quad (3.9)$$

and

$$E[G(q)|D, M] \approx \frac{1}{N} \sum_{i=1}^N G(q^{(i)}) \quad (3.10)$$

respectively, where $q^{(i)} \equiv q(\underline{\theta}^{(i)})$

3.3 Fast Computing Techniques for Large Order Finite Element Models

3.3.1 Component Model Synthesis for Parameter Estimation in Structural Dynamics

At the system level, dynamic reduction techniques such as CMS can be implemented with Bayesian uncertainty quantification and propagation framework in order to alleviate the computational burden associated with each model run in the re-analyses required in the optimization and stochastic simulation methods. CMS techniques have been successfully employed for model reduction in optimization and stochastic simulation algorithms involved in model updating [15, 16]. CMS techniques [7] divide the structure into components with mass and stiffness matrices that are reduced using fixed-interface and constrained modes. Dividing the structure into components and reducing the number of physical coordinates to a much smaller number of generalized coordinates certainly alleviates part of the computational effort. However, at each iteration or TMCMC sampling

point one needs to re-compute the eigen-problem and the interface constrained modes for each component. This procedure is usually a very time consuming operation and computationally more expensive than solving directly the original matrices for the eigenvalues and the eigenvectors. It was recently shown [8] that for certain parameterization schemes for which the mass and stiffness matrices of a component depend linearly on only one of the free model parameters to be updated, often encountered in finite element model updating formulations, the full re-analyses of the component eigen-problems are avoided. The eigenproperties and the interface constrained modes as a function of the model parameters can be computed inexpensively from the eigenproperties and the interface constrained modes that correspond to a nominal value of the model parameters.

Specifically let Δ_j be the set of structural components that depend on the j -th parameter θ_j . Consider the case for which the stiffness matrix of a component $s \in \Delta_j$ depends linearly θ_j and the mass matrix is independent of θ_j , i.e. $K_{(s)} = \bar{K}_{(s)}\theta_j$ and $M_{(s)} = M_0^{(s)}$. It can be readily derived that the stiffness and mass matrices of the Craig-Bampton reduced system admits the representation

$$\hat{K}_{CB} = \hat{K}_0^{CB} + \sum_{j=1}^{N_\theta} \hat{K}_j^{CB} \theta_j \quad \text{and} \quad \hat{M}_{CB} = \hat{M}_0^{CB} \quad (3.11)$$

where the coefficient matrices \hat{K}_0^{CB} , \hat{K}_j^{CB} and \hat{M}_0^{CB} in the expansion (3.11) are assembled from the component stiffness and mass matrices. It is important to note that the assembled matrices \hat{K}_0^{CB} , \hat{K}_j^{CB} and \hat{M}_0^{CB} of the Craig-Bampton reduced system in the expansion (3.11) are independent of the values of θ . In order to save computational time, these constant matrices are computed and assembled once and, therefore, there is no need this computation to be repeated during the iterations involved in optimization or TMCMC sampling algorithms for model updating due to the changes in the values of the parameter vector θ . This is an important result which saves substantial computational effort since it avoids (a) re-computing the fixed-interface and constrained modes for each component, and (b) assembling the reduced matrices from these components. The formulation guarantees that the reduced system is based on the exact component modes for all values of the model parameters.

The aforementioned formulation can readily be extended to treat the more general case in which the stiffness and mass matrices of a component depends nonlinearly on a single parameter, that is $K_{(s)} = \bar{K}_{(s)}f(\theta_j)$ and $M_{(s)} = \bar{M}_{(s)}\rho(\theta_j)$, where $f(\theta_j)$ and $\rho(\theta_j)$ are scalar nonlinear functions of a parameter. In this case the linear representation (3.11) is no longer applicable for such components. However, the reduced stiffness and mass matrices for each component as a function of the model parameters can be readily obtained from the eigen-properties and constrained interface modes obtained from a single analysis for a nominal value of the component parameter θ_j . It turns out that substantial computational savings arise from the fact that the re-analyses of the fixed-interface and constrained modes for each component required at each iteration or TMCMC sampling point is completely avoided. In this general case, the reduced stiffness and mass component matrices have to be re-assembled in order to derive the Craig-Bampton reduced system matrices. Similar to the linear case [8], the computational demands in FE model updating formulations are again substantially reduced without compromising the solution accuracy.

3.3.2 Surrogate Models

At the level of the TMCMC algorithm, surrogate models can be used to reduce the computational time by avoiding the full model runs at a large number of sampling points in the parameters space. This is done by exploiting the function evaluations that are available at the neighbour points from previous full model runs in order to generate an estimate at a new sampling point in the parameter space. Surrogate models are well-suited to be used with MCMC algorithms, including the TMCMC algorithm [6]. The kriging technique [17] is used to approximate the function evaluation at a sampling point using the function evaluations at neighbor points in the parameter space. To ensure a high quality approximation, certain conditions are imposed in order a surrogate estimate be accepted. Specifically, the estimate is accepted based on a minimum number of neighbour design points that depend on the dimension of the uncertain parameter space. The surrogate point has to belong to the convex hull of the design points so that an interpolation is performed, while extrapolations are prohibited. The neighbour design points are selected as the ones closest to the surrogate estimate and also within the hyper-ellipse of the TMCMC proposal covariance matrix scaled to include the minimum number of design points. The estimate is also accepted based on local optimality conditions for the selected surrogate scheme, guaranteeing that the error in the surrogate estimate provided by the kriging technique is smaller than a user-defined value. Details of the integration of the kriging technique within the TMCMC algorithm can be found in [9]. An order of magnitude reduction in the number of full model runs involved in TMCMC algorithm has been reported which results in additional computational savings.

3.3.3 Parallel Computing Algorithms

At the computer hardware level, high performance computing (HPC) techniques can be used to reduce the computational time. Most MCMC algorithms involve a single Markov chain and are thus not parallelizable. In contrast, the TMCMC algorithm involves a large number of independent Markov chains that can run in parallel. Thus, the TMCMC algorithm is very-well suited for parallel implementation in a computer cluster [9]. Specifically, parallelization is activated at every stage of the TMCMC algorithm exploiting the large number of short, variable length, chains that need to be generated starting from the leader samples determined from the TMCMC algorithm at the particular stage. Static and dynamic scheduling schemes can be conveniently used to optimally distribute these chains in a multi-host configuration of complete heterogeneous computer workers. The static scheduling scheme distributes the chains in the workers using a weighted round-robin algorithm so that the number of likelihood evaluations is arranged to be the same for each computer worker. The static scheduling scheme is computationally efficient when the computational time for a likelihood evaluation is the same independently of the location of sample in the parameter space as well as when surrogate estimates are not activated. The dynamic scheduling scheme is more general, ensuring a more efficient balancing of the loads per computer worker in the case of variable run time of likelihood function evaluations and unknown number of surrogates activated during estimation. Specifically, each worker is periodically interrogated at regular time intervals by the master computer about its availability and samples from TMCMC chains are submitted to the workers on a first come first serve basis to perform the likelihood function evaluations so that the idle time of the multiple workers is minimised. Details of the parallel implementation of the TMCMC algorithm are given in [9].

3.4 Application on Finite Element Model Updating of a Bridge

The efficiency of the proposed fast computing tools in the Bayesian framework is demonstrated by updating a FE model of the Metsovo bridge (Fig. 3.1a) using simulated modal data. A detailed FE model of the bridge is created using 3-dimensional tetrahedron quadratic Lagrange FEs. An extra coarse mesh, chosen to predict the lowest 20 modal frequencies and mode shapes of the bridge, results in a minimum 97,636 FEs and 562,101 DOF. The size of the elements in the extra coarse mesh is the maximum possible one that can be considered, with typical element length of the order of the thickness of the deck cross-section.

Let ω_c be the cut-off frequency which represents the highest modal frequency that is of interest in FE model updating. Herein, the cut-off frequency is selected to be equal to the 20th modal frequency of the nominal model. That is $\omega_c = 4.55$ Hz. For demonstration purposes, the bridge is divided into nine physical components with eight interfaces between components as shown in Fig. 3.1b. For each component it is selected to retain all modes that have frequency less than $\omega_{\max} = \rho \omega_c$, where the ρ values affect computational efficiency and accuracy of the CMS technique. The total number of internal DOFs before the model reduction is applied and the number of modes retained for various ρ values are given in Table 3.1. For the case $\rho = 8$, a total of 286 internal modes out of the 558,801 are retained for all 9 components. The total number of DOFs of the reduced model is 3,586 which consist of 286 fixed interface generalized coordinates and 3,300 constraint interface DOFs for all components. It is clear that a two orders of magnitude reduction in the number of DOFs is achieved using CMS.

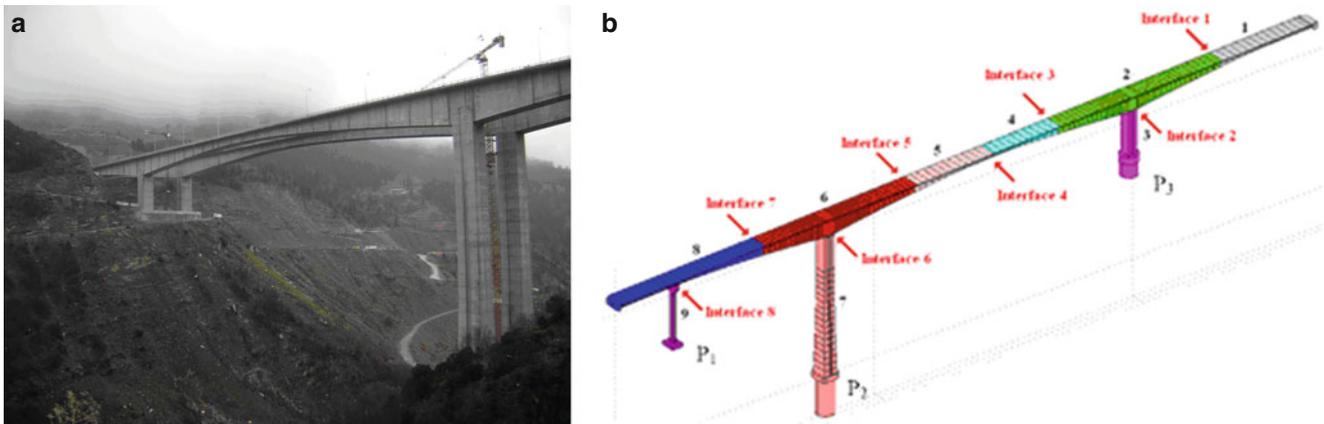


Fig. 3.1 (a) Metsovo bridge, (b) components of FE model of the bridge

Table 3.1 Number of DOF and percentage modal frequency error for the full (unreduced) and reduced models

	Full model	Reduced model (Retained modes)					
		$\rho = 8$	$\rho = 5$	$\rho = 2$	$\rho = 8$ $v = 200$	$\rho = 5$ $v = 200$	$\rho = 2$ $v = 200$
Internal DOF	558,801	286	100	31	286	100	31
Interface DOF	3,300	3,300	3,300	3,300	306	306	306
Total DOF	562,101	3,586	3,400	3,331	592	406	337
Highest percentage error (%)	0.00	0.02	0.17	1.10	0.20	0.30	1.20

Table 3.1 also shows the fractional error between the modal frequencies computed using the complete FE model and the ones computed using the CMS technique for $\rho = 2, 5$ and 8 . It is seen that the error fall below 0.02% for $\rho = 8$, 0.17% for $\rho = 5$ and 1.10% for $\rho = 2$. A very good accuracy is achieved for the case of $\rho = 5$.

For the specific application, a large number of generalized coordinates for the reduced system arises from the interface DOFs. A further reduction in the number of generalized coordinates for the reduced system can be achieved by retaining only a fraction of the constrained interface modes [18]. For each interface, it is selected to retain all modes that have frequency less than $\omega_{\max} = v\omega_c$, where v is user and problem dependent. Results are computed for $v = 200$. The number of interface modes retained is given in Table 3.1. It can also be seen that the fractional error for the lowest 20 modes of the structure fall below 1.20% for $v = 200$. In particular, the value of $v = 200$ and $\rho = 5$ gives sufficiently accurate results and the number of retained interfaces modes for all interfaces is 306. The reduced system has 406 DOFs from which 100 generalized coordinates are fixed-interface modes for all components and the rest 306 generalized coordinates are constrained interface modes. Using CMS, the number of generalized coordinates is drastically reduced.

For demonstration purposes, the FE model is parameterized using five parameters associated with the modulus of elasticity of one or more structural components shown in Fig. 3.1b. Specifically, the first two parameters θ_1 and θ_2 account respectively for the modulus of elasticity of the pier components 3 and 7 of the bridge. The parameter θ_3 accounts for the modulus of elasticity of the components 1 and 2 of the deck, the parameter θ_4 accounts for the components 4 and 5, while the parameter θ_5 accounts for the components 6 and 8. The component 9 is not parameterized.

The estimation of the parameter values and their uncertainties of the FE model is based on modal frequencies and mode shapes. Simulated, noise contaminated, measured modal frequencies and mode shapes are generated by adding a 1 and 3% Gaussian noise to the modal frequencies and modeshape components, predicted by the nominal non-reduced FE models. The added Gaussian noise reflects the differences observed in real applications between the predictions from a model of a structure and the actual (measured) behavior of the structure. 38 sensors are placed on the bridge to monitor vertical and transverse accelerations. The measured data contain the values of the ten lowest modal frequencies and modeshapes. The model parameters are introduced to scale the nominal values of the properties that they model so that the value of the parameters equal to one corresponds to the nominal value of the FE model.

The model updating is performed using the stochastic simulation algorithm TMCMC with the following settings of the TMCMC parameters: $\text{tolCov} = 1.0$, $\beta = 0.2$ and 1,000 samples per TMCMC stage [6]. The number of FE model runs for the five-parameter model class depends on the number of TMCMC stages which was estimated to be 19. The resulting number of FE model re-analyses are 19,000. The parallelization features of TMCMC [9] were also exploited, taking advantage of the available four-core multi-threaded computer unit to simultaneously run eight TMCMC samples in parallel. For comparison purposes, the computational effort for solving the eigenvalue problem of the original unreduced FE model is approximately 139 s. Multiplying this by the number of 19,000 TMCMC samples and considering parallel implementation in a four-core multi-threaded computer unit, the total computational effort for the model class is expected to be of the order 7 days. In contrast, for the reduced-order models for $\rho = 8$, the computational demands for running the model class are reduced to approximately 13 h (759 min), while for the reduced-order models for $\rho = 8$ and $v = 200$ these computational demands are drastically reduced to 14 min. It is thus evident that a drastic reduction in computational effort for performing the structural identification based on a set of monitoring data is achieved from approximately 7 days for the unreduced model class to 14 min for the reduced model classes corresponding to $\rho = 8$ and $v = 200$, without compromising the predictive capabilities of the proposed parameter estimation methodology. This results in a factor of over 500 reduction in computational effort. It should be noted that kriging technique further reduces the computational effort by approximately one order of magnitude so that the updating of the 562,101 DOF finite element model, requiring 19,000 model runs, can be performed in 2 min which is a remarkable reduction in computational effort.

3.5 Conclusions

Asymptotic approximations and stochastic simulation algorithms (e.g. the TMCMC algorithm) used in Bayesian model uncertainty quantification, calibration and propagation requires a large number of FE model simulation runs. For large size FE models with hundred of thousands or even million DOFs and localized nonlinearities, the computational demands involved in the optimization or TMCMC sampling algorithms may be excessive. Drastic reductions can be achieved at the system, algorithm and computer equipment level. At the system level, CMS techniques that exploit certain schemes often encountered in FE model parameterization are shown to be effective in completely avoiding the large number of eigen-problem re-analyses within the components or interfaces, required during the application of the optimization or TMCMC sampling algorithms. Thus parameterization consistent CMS techniques result in drastic reduction of the computational effort. At the level of the algorithm, surrogate models are well adapted to the TMCMC algorithm for significantly reducing the number of full model runs required, without sacrificing the accuracy in the surrogate estimates. At the computer hardware level, parallel computing algorithms are also very well suited to be used with TMCMC algorithm to efficiently distribute the computations in available multi-core CPUs. Application of the framework to uncertainty calibration of a structural model using vibration measurements was emphasized in this work. The method has also been successfully applied to structural health monitoring for identifying the location and severity of damage [8]. The fast computing techniques implemented within the Bayesian framework can also be used for updating robust model-based predictions and reliability given monitoring data.

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