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Efficient surrogate-based optimization using reduced order models by moment matching coupled with kriging

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Structured Abstract.

Purpose – Performing dynamic simulation and optimization of electromagnetic systems can be very time consuming and even prohibitively slow when used in optimization processes. This paper contains a new methodology that couples Model Order Reduction (MOR) with a Response Surface Methodology (RSM) to greatly reduce the computational time. The methodology is validated by optimizing the capacitors placement on a laminated bus bar.

Design/methodology/approach – The proposed methodology uses Moment Matching (MM) as a Model Order Reduction technique to perform very fast computation of objective functions. These results are used as input by a Kriging interpolations algorithm to create an adaptive Response Surface (RS). Optimization is performed based on the Expected Improvement (EI). To guarantee that the objective functions computed by the Reduced Order Models are accurate, an adaptive reduction schema is developed.

Findings – The methodology has been able to greatly reduce the optimization time. An adaptive Model Order Reduction schema has been successful in producing accurate models for different parameters demanded by the optimization process.

Research limitations/implications – Not all systems are eligible to be used by the proposed methodology. They are assumed to be writable in the form of a generalized state space. Therefore, only linear systems are eligible.

Originality/value – Two different techniques for accelerating computational time in optimization have been combined. A method to perform adaptive Model Order Reduction has been used to guarantee accuracy, allowing the connection of the methods.

Keywords: Dynamic Model Optimization, Kriging, Model Order Reduction, Moment Matching and Optimization.

1. INTRODUCTION

The development of physical modelling, and more specifically electromagnetic modelling, has greatly evolved in the last decades, allowing high-fidelity simulation of a myriad of physical systems. Part of this development may be attributed to the advances in the Finite Element Method (FEM) (Rao, 2017) and other formulations such as the Partial Element Equivalent Circuit (PEEC) (Nitsch, et al., 2009).

However, directly applying these techniques to complex systems or demanding a very high accuracy, may result in a prohibitive computational burden. This is especially problematic when many simulations must be performed, such as in optimizations loops (AO Leite, et al., 2016). Once that each individual simulation is quite expensive, many authors have used surrogate techniques to reduce the computational burden (Jones, et al., 1998) (Knowles, 2006). Approaches such as Space Mapping (Gong, et al., 2018) and Kriging (Olea, 2012) have been especially successful. The latter is capable of producing a Response Surface (RS) based on a few simulation results. One of its main advantages is the possibility to estimate the prediction error at unsampled points.

Complementary, Model Order Reduction (MOR) is a technique that can be used to reduce the simulation burden of complex dynamical system (Antoulas, 2005). It is an efficient method to mitigate this problem, producing easy to simulate and accurate models in a fraction of the computational time. These models can be obtained from the simulation of the High-Fidelity Model (HFM) for a short period of time (Willcox & Peraire, 2002), by removing states from the system that are poorly controllable and reachable (Moore, 1981), by matching moments of the HFM transfer function (Freund, 2000), among others.

In this paper, the coupling of Moment Matching (MM) technique with Kriging is proposed. In doing so, one must be sure that the results produced by the Reduced Order Models (ROM) are accurate even when the optimization algorithm drastically vary the parameters of the model during its search. Therefore, an adaptive reduction procedure is presented. The methodology has been tested on the problem of placing capacitors on a laminated bus bar, obtaining very encouraging results.

The paper is divided as follows. The MOR procedure and the Response Surface Methodology (RSM) are described, respectively, in Sections 2 and 3. The electromagnetic model used to validate the optimization process is detailly described in Section 4. The results and conclusions are shown in Sections 5 and 6, respectively.

2. ADAPTIVE MODEL ORDER REDUCTION

It is assumed that the High-Fidelity Model can be written in the form of a dynamic linear system in descriptor form, as in in (1). In these equations: $x \in \mathbb{R}^n$, $u \in \mathbb{R}^i$ and $y \in \mathbb{R}^o$. These vectors are, respectively, the state and the inputs and outputs of the system. Consistently, $A, E \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times i}$ and $C \in \mathbb{R}^{o \times n}$. Note that n , i and o are, respectively, the dimension of the system, the number of inputs and the number of outputs.

$$\begin{cases} E\dot{x} &= Ax + Bu \\ y &= Cx \end{cases} \quad (1)$$

Many of the reduction methods can be cast into a similar mathematical formulation, known as the projection framework (Benner, et al., 2015). It consists in the projection of the state vector of the HFM into a subspace of smaller dimension q denoted by \mathcal{V} . The result of this process can be seen in (2). In these equations, $V \in \mathbb{C}^{n \times q}$ and $\text{span}\{V\} = \mathcal{V}$.

$$\begin{cases} V^T E V \dot{x}_r &= V^T A V x_r + V^T B u \\ y_r &= C V x_r \end{cases} \quad (2)$$

The matrix V should not be chosen arbitrarily. Different methods use distinct manners of computing the matrix V (Antoulas, 2005). In general, it is expected that (3) holds.

$$x \approx V x_r \quad (3)$$

2.1. Moment Matching

Among the different MOR methods, Moment Matching has been especially successful in reducing electromagnetic models and electrical circuits (Freund, 2004). This method produces ROM whose transfer function moments match those of the HFM up to a given order in a finite set of expansion points chosen by the

user. Although mathematically distinct, this process is similar to a Taylor polynomial fitting, but with more than one expansion point.

A sufficient condition for moment matching at the point $s_0 = j2\pi f_0$ up to an order k and frequency f_0 is shown in (4) (Freund, 2004). Direct computation of V by this equation is not advised due to severe numerical problems. One should use an Arnoldi process instead (Arnoldi, 1951).

$$\text{span}\{V\} \supseteq [(A - s_0 E)^{-1} E]^i (A - s_0 E)^{-1} B \quad i = 0, \dots, k \quad (4)$$

Note that the different expansion points must be chosen by the user. Using the same set of points for different systems or for the same system but with different parameters may not produce accurate results once that the frequency response is different. Therefore, a process to adaptively place the expansions points is needed in an optimization loop.

2.2. Adaptive placing of expansion points

The problem of optimally placing expansion points is not new in the Moment Matching Literature (Paquay, et al., 2016) (Lein, et al., 2015) (AO Leite, et al., 2016). The method presented in this section has the advantage of being very simple and working without modification for Many Inputs Many Outputs (MIMO) systems.

The process of adaptively choosing expansion points is guided by a greedy algorithm that aims at reducing a specific residue. It may be derived by taking the Laplace transform of the first equation in (1), which results in (5).

$$(Es - A)x = B \mathcal{L}\{u\} \quad (5)$$

In choosing the input as being an impulse and applying the approximation in (3), the equation for the residue $r \in \mathbb{C}^n$ is given by (6). Note that for each frequency there will be a different residue vector.

$$(Es - A)Vx_r - B = r \quad (6)$$

By the use of a metric, one can determine the frequency of greatest residue, location of the new expansion point. If the maximum residue is less than a given threshold, the process stops. Note that the process of computing r requires x_r . However, its computation is very fast due to its small dimension and due to the existing fast frequency sweeping algorithms (Laub, 1981).

One constructs the first ROM using an expansion point (empirically with two moments) at both extremes of a frequency interval provided by the user. Algorithm 1 summarizes the iterative process which add the required other expansion points (empirically with one moment).

Algorithm 1- Model Order Reduction

Input \mathcal{M} (High-Fidelity Model), $[f_l, f_u]$ (Frequency interval), ϵ (threshold)
Output \mathcal{M}_r (Reduced Order Model)

```

1   $f_0 \leftarrow \{f_l, f_u\}$ 
2   $R_{min} \leftarrow \infty$ 
3  While  $R_{min} > \epsilon$  do
4       $\mathcal{M}_r \leftarrow \text{Reduce Model } (\mathcal{M}, f_0)$ 
5       $X_r \leftarrow \text{Simulation } (\mathcal{M}_r)$ 
6       $f_0 = \text{argmin } |(j 2 \pi f E - A) \vee X_r(f) - B|$ 
7       $R_{min} \leftarrow |(j 2 \pi f_0 E - A) \vee X_r(f_0) - B|$ 
8  End
```

3. RESPONSE SURFACE METHODOLOGY WITH KRIGING

One way of performing optimization with ROMs is to construct ROM that keep the dependency on the design parameters. This is known as Parametric Model Order Reduction (PMOR) (Amsallem, 2010). However, this technique assumes that the number of equations for the different linear systems is the same. This poses problems when dealing with systems whose mesh vary adaptively.

Once that the objective function is a real value extracted from the dynamical system, one can apply techniques such as Kriging to overcome this problem. Originally, it has been used in geology to determine the distribution of some mineral or soil property in a given area when only a few samples are known (Olea, 2012). Due to its powerful interpolation capability and the possibility to estimate the error, it has been used by researchers as a way to reduce computational burden in optimization processes (Jones, et al., 1998).

Assume that there is an objective function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, such that d is the number of decision variables. Each evaluation of f is potentially very time consuming and therefore, should be reduced as much as possible. Kriging can be used to compute an RS to estimate the objective function at unsampled regions. Further improvements in the optimization process are done, as explained in the following paragraphs.

Given only the box constraints of the problem, one starts by sampling the design space in a given number of points. A space-filling technique such as a Latin Hypercube Sampling (LHS) can be used (Montgomery, 2017). MOR is used to accelerate this process for each one of these points. Having these data, a model can be fit and used as an approximation of the objective function in unsampled points.

An iterative process of refining the sampling and searching for points that may improve the current best result is performed. Following the idea presented in (Jones, et al., 1998), new samples are chosen by maximization of the Expected Improvement (EI) (Jones, 2001).

Therefore, an internal optimization cycle is performed at each refinement step. The burden of this process is acceptable, once that computing a prediction is much faster than computing the objective function which require the construction of a ROM. The whole process described in this section is shown in Figure 1. Note that for each computation of the objective function, a MOR is performed (time consuming but far less than HFM simulation). The ROM is simulated in time or frequency domain (very fast) and a feature extraction is performed to obtain the scalar criteria (mean value, maximal value, average differences, etc.).

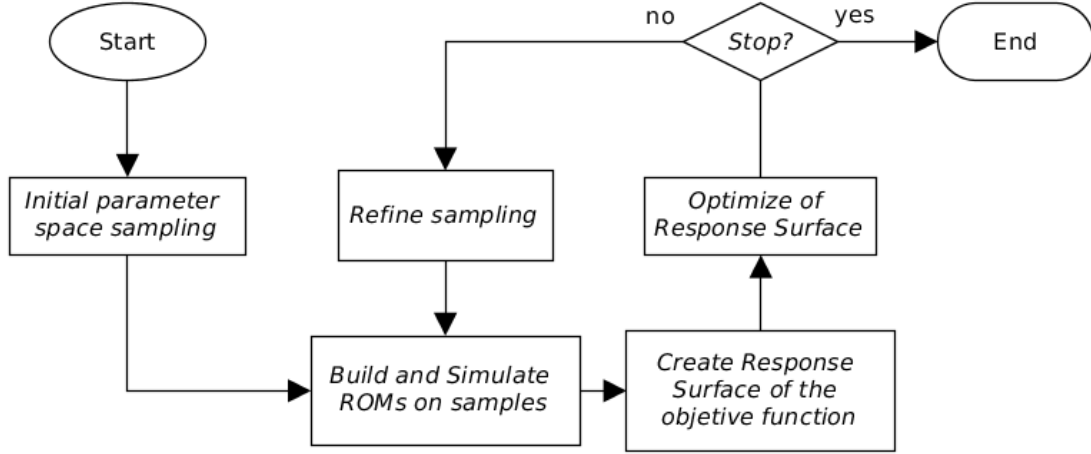


Figure 1 - Flowchart of the optimization process with a surrogate model

4. APPLICATION

The proposed methodology has been validated by its application of the design optimization of an electromagnetic device (Kuwabara, et al., 2016). It consists in a laminated bus bar with four capacitors, a load and a source. A drawing of the system is shown in Figure 2.

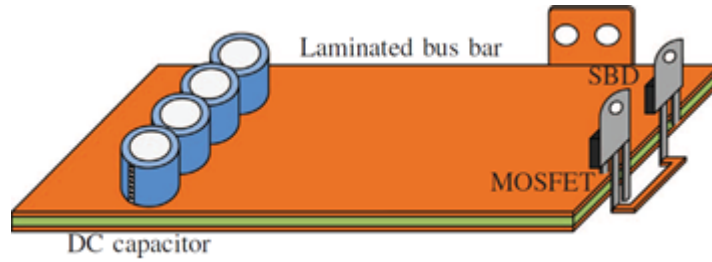


Figure 2 - Drawing of the laminated bus bar. Adapted from the original (Kuwabara, et al., 2016)

During the lifetime of the laminated bus bar, the different capacitors will be stressed by different currents. This may lead to premature failure of one of them. The optimization process seeks to position the four capacitors in a way that the current is uniformly distributed on the whole operational frequency range.

The plates are made of copper and the capacitance of each capacitor is 1 mF. The load used in this example has been selected as a series association of a 10 Ω resistance with a 1 μ H inductance.

The electromagnetic model has been obtained by coupling the discrete capacitors, source and load to the circuit obtained by applying an unstructured PEEC formulation to the system (Siau, 2016). The objective function which requires performing frequency simulations, should be prohibitively time consuming if using HFM. Therefore, the proposed methodology based on MOR and RSM has been applied.

5. RESULTS

The optimization algorithm aims at minimizing the modulus of the pairwise difference of the capacitor currents in the frequency range from 10^3 rad/s to 10^7 rad/s. The objective function can be seen explicitly in (7).

$$f = \frac{1}{2 n_p} \sum_{k=1}^4 \sum_{l=1}^4 |I_k - I_l| \quad (7)$$

In this equation, n_p represents the number of sample points chosen in the frequency range, and the vectors $I_k \in \mathbb{C}^{n_p}$ are obtained by the simulation of the model for the current capacitor placement.

It is not possible to place the capacitors too close together due to constructive difficulties. Therefore, there is one restriction to the problem that penalizes solutions whose capacitors are too close together. The penalty term p that is added to the objective function is given by (8). Additional box constraints have been added to ensure that no capacitor is positioned outside the surface of the plates.

$$p = 100 \sum_{k=1}^4 \sum_{l>k}^4 \max \left\{ 0 \quad ; \quad 16 \times 10^{-3} - \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \right\} \quad (8)$$

The High-Fidelity Model has order 4688 and its simulation takes around 900 seconds. The Reduced Order Models all have order less than 30. The reduction process takes around 55 seconds per design configuration, but the frequency simulation and objective function extraction can be made in milliseconds.

The overall optimization process takes about three hours. The initial Kriging model has been built with 80 sampling points and 120 new refinement points have been added adaptively in the process. This means building and simulating 200 ROMs. If the same number of function calls were made using the HFM, the process would have taken more than 50 hours, leading to a speed increase factor of 16 on this application.

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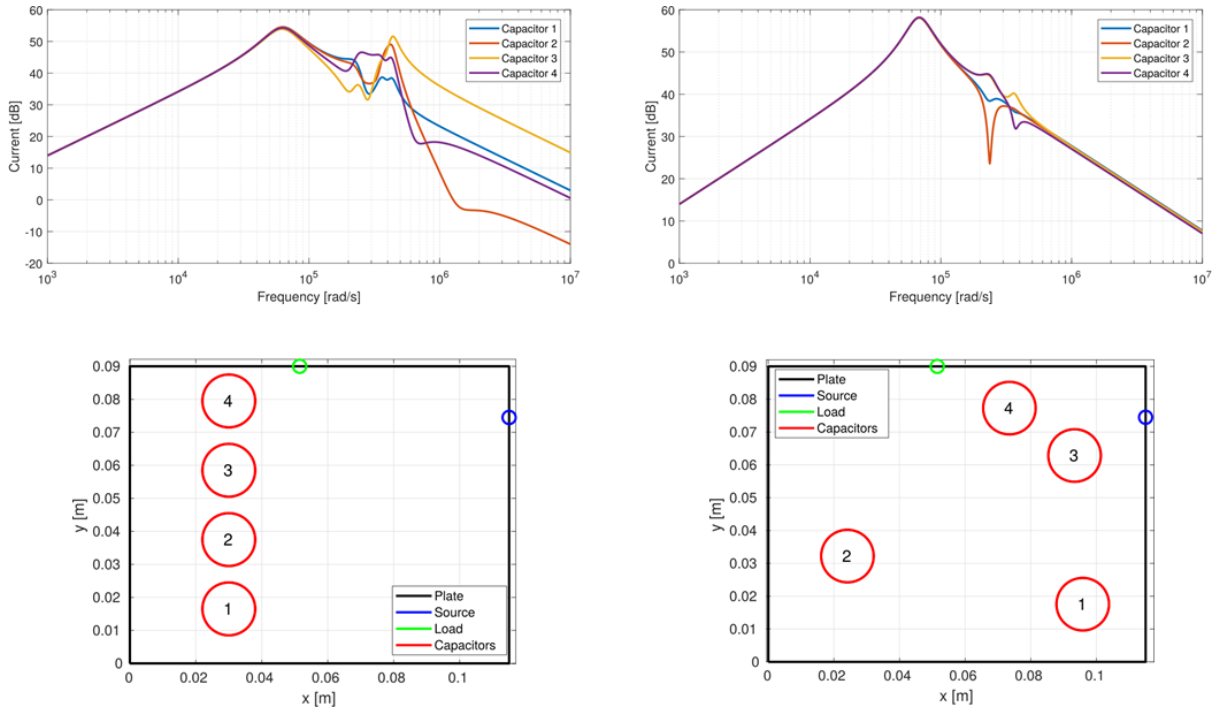


Figure 3 - Capacitors positioning and currents before (left) and after (right) the optimization process

6. CONCLUSIONS

A method to couple Model Order Reduction with optimization using a Response Surface Methodology with Kriging has been presented. To guarantee that the Reduced Order Model is accurate independently of the parameters required by the optimization algorithm, an adaptive method for placing the expansion points has been developed.

The method has been applied to a problem of placing capacitors in a laminated bus bar. The results show that the method has found a suitable solution with much less computational time that would be needed if the High-Fidelity Model had been applied. Moreover, Moment Matching method does not require the HFM simulation, so it is also a way to simulate and optimize HFM that cannot be simulated due to time or computer memory limitations.

There are, however, some limitation to the proposed methodology based on Moment Matching since this method is only capable of reducing linear models. Therefore, further research must consider the case of nonlinear systems.

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