Design Optimization of Sonnet-Simulated Structures Using Space Mapping and Kriging

Slawomir Koziel

Engineering Optimization & Modeling Center, School of Science and Engineering,
Reykjavik University, 101 Reykjavik, Iceland
koziel@ru.is

Abstract: An efficient algorithm for design optimization of structures simulated using Sonnet ***em*** is discussed. Our approach uses coarse-discretization model of the structure of interest that is optimized on a coarse grid using pattern search. Space mapping optimization is then performed with the underlying surrogate model created using kriging interpolation of coarse-discretization Sonnet model data. The design of two microstrip filters is considered for illustration.

Keywords: Computer-Aided Design (CAD), Electromagnetic Simulation, Space Mapping, Microwave Design, Kriging Interpolation.

1. Introduction

Electromagnetic (EM) simulation has become one of the fundamental tools in the microwave design process. While initially used mostly for design verification, EM simulation is now commonly used to adjust geometry and/or material parameters of the device of interest so that it satisfies given performance requirements. In practice, such an adjustment process—also referred to as design closure [1]—is performed through repetitive parameters sweeps (typically, one parameter at a time), guided by expert knowledge. This is a laborious process which does not guarantee optimal results. Therefore, automated simulation-driven design is highly desirable. Unfortunately, it faces some serious difficulties, the most important of which is high computational cost of accurate EM evaluation. As a result, the use of conventional design optimization techniques that require large number of EM simulations (e.g., gradient-based methods) may be impractical.

Computationally efficient EM-simulation-driven design closure can be realized using surrogate-based optimization (SBO) [2]. The basic component of an SBO algorithm is a surrogate model - a computationally cheap representation of the structure under consideration (high-fidelity model). The surrogate is iteratively updated and re-optimized in order to yield a satisfactory design of the original structure [3]. Surrogate models can be constructed by approximating sampled high-fidelity model data [2], [4] or by suitable correction of a physically-based low-fidelity (or "coarse") model, e.g., an equivalent circuit [5].

The most successful techniques in microwave engineering exploiting physically-based surrogates are (SM) [5]-[8] and various forms of tuning [1], [9], [10] and tuning SM [11], [12]. The tuning approaches are particularly suited to be used with Sonnet ***em*** [13] because of its co-calibrated ports technology [1]. Other methods include various response correction techniques such as manifold mapping [14], adaptive response correction [15] or shape-preserving response prediction [16].

Space mapping seems to be the most generic approach; however, its efficiency heavily depends on the quality of the coarse model [17]. Also, SM normally requires that the coarse model is very fast. These requirements are often contradictory. In particular, fast coarse models (e.g., equivalent circuits) are usually not quite accurate, whereas accurate models (e.g., coarse-discretization EM simulations) are relatively expensive. In [18], an algorithm was proposed that uses space mapping as well as coarse-discretization Sonnet simulations and shape-preserving response prediction (SPRP) [16] to create the coarse model. This methodology proved very efficient, however, SPRP assumes that the coarse and fine model response shapes must be similar (in terms of specifically defined characteristic points) for all designs considered during the optimization run. This limits the range of applications of this methodology and requires that the set of characteristic points is individually defined on case to case basis.

In this paper, we adopt similar approach which overcomes the aforementioned limitations of [18]. The space mapping algorithm is again used as an optimization engine. However, the coarse model is constructed through kriging interpolation [4] of coarse-discretization Sonnet simulations. While kriging requires more data points than SPRP to create the model, it is more general and easier to implement. Our technique is demonstrated through the design of two microstrip filters.

2. Design Optimization Coarse-Discretization Sonnet Simulations, Kriging and Space Mapping

A. Design Optimization Problem

The design problem is formulated as a nonlinear minimization problem of the following form:

$$\boldsymbol{x}_f^* \in \arg\min_{\boldsymbol{x}} U(\boldsymbol{R}_f(\boldsymbol{x})), \tag{1}$$

Here, $\boldsymbol{R}_f(\boldsymbol{x}) \in R^m$ is a response vector of a structure of interest, e.g., $|S_{21}|$ at m frequencies; $\boldsymbol{x} \in R^n$ is a design variable vector; U is a scalar merit function, e.g., a minimax function with upper/lower specifications; $\boldsymbol{x}_f^*$ is the optimal design to be determined. Here, $\boldsymbol{R}_f$ is evaluated using Sonnet ***em*** with a $g_{h.f} \times g_{v.f}$ grid.

B. Coarse-Discretization Model and Initial Optimization Stage

The optimization technique introduced here exploits a coarse-discretization model $\boldsymbol{R}_{cd}$, also evaluated using Sonnet ***em***. The model $\boldsymbol{R}_{cd}$ exploits a grid $g_{h.c} \times g_{v.c}$ so that $g_{h.c} > g_{h.f}$ and $g_{v.c} > g_{v.f}$.

The model $\boldsymbol{R}_{cd}$ is optimized on the grid $g_{h.c} \times g_{v.c}$ using a pattern search algorithm [20] in order to find a design $\boldsymbol{x}^{(0)}$ that will be used as a starting point for the next optimization stage. The resolution of this initial optimization stage is limited by the coarseness of the grid $g_{h.c} \times g_{v.c}$, however, for the same reason, the computational cost of finding $\boldsymbol{x}^{(0)}$ is low and typically corresponds to a few evaluations of the fine model $\boldsymbol{R}_f$.

C. Coarse Model Construction Using Kriging Interpolation

In this work, we use space mapping algorithm as an optimization engine (see Section 2.*D*). Space mapping requires that the underlying coarse model is fast and easy to optimize. Neither of these conditions is satisfied for the coarse-discretization model $\boldsymbol{R}_{cd}$ described in Section 2.*B*. Therefore, we create the coarse model as a response surface approximation model of the sampled coarse-discretization Sonnet simulation data. This allows us to reduce the computational overhead of the optimization process because, after the initial setup, the model $\boldsymbol{R}_{cd}$ is not evaluated during the space mapping algorithm run. Also, the kriging-based coarse model is smooth and thus easy to optimize.

The coarse model $\boldsymbol{R}_c$ is set up in the vicinity of $\boldsymbol{x}^{(0)}$ defined by the grid size of the coarse-discretization model $\boldsymbol{R}_{cd}$. Let $X_B = \{\boldsymbol{x}^1, \boldsymbol{x}^2, \ldots, \boldsymbol{x}^N\}$ denote a base set, such that the responses $\boldsymbol{R}_{cd}(\boldsymbol{x}^j)$ are known for $j = 1, 2, \ldots, N$. The base designs are assigned using Latin Hypercube Sampling algorithm [21]. Let $\boldsymbol{R}_{cd}(\boldsymbol{x}) = [R_{cd\,1}(\boldsymbol{x}) \ldots R_{cd.m}(\boldsymbol{x})]^T$ (components of the model response vector may correspond to certain parameters, e.g., $|S_{21}|$ evaluated at m frequency points).

Here, we use ordinary kriging [4] that estimates deterministic function f as $f_p(\boldsymbol{x}) = \mu + \varepsilon(\boldsymbol{x})$, where μ is the mean of the response at base points, and ε is the error with zero expected value, and with a correlation structure being a function of a generalized distance between the base points. We use a Gaussian correlation function of the form

$$R(\boldsymbol{x}^i, \boldsymbol{x}^j) = \exp\left[\sum_{k=1}^{N} \theta_k \,|\, x_k^i - x_k^j \,|^2\right], \tag{2}$$

where θ_k are unknown correlation parameters used to fit the model, while x_k^i and x_k^j are the kth components of the base points $\boldsymbol{x}^i$ and $\boldsymbol{x}^j$.

The kriging-based coarse model $\boldsymbol{R}_c$ is defined as

$$\boldsymbol{R}_c(\boldsymbol{x}) = \left[R_{c\,1}(\boldsymbol{x}) \ \ \ldots \ \ R_{c\,m}(\boldsymbol{x})\right]^T, \tag{3}$$

where

$$R_{c\,j}(\boldsymbol{x}) = \bar{\mu}_j + \boldsymbol{r}^T(\boldsymbol{x})\boldsymbol{R}^{-1}(\boldsymbol{f}_j - \boldsymbol{1}\bar{\mu}_j). \tag{4}$$

Here $\boldsymbol{1}$ denotes an N-vector of ones,

$$\boldsymbol{f}_j = [R_{cd\,j}(\boldsymbol{x}^1) \ \ldots \ \ldots R_{cd\,j}(\boldsymbol{x}^N)]^T, \tag{5}$$

$\boldsymbol{r}$ is the correlation vector between the point $\boldsymbol{x}$ and base points

$$\boldsymbol{r}^T(\boldsymbol{x}) = [R(\boldsymbol{x},\boldsymbol{x}^1) \ \ldots \ \ldots R(\boldsymbol{x},\boldsymbol{x}^N)]^T, \tag{6}$$

whereas $\boldsymbol{R}$ is the correlation matrix between the base points

$$\boldsymbol{R} = \begin{bmatrix} R(\boldsymbol{x}^1,\boldsymbol{x}^1) & R(\boldsymbol{x}^1,\boldsymbol{x}^2) & \text{[redacted]} & R(\boldsymbol{x}^1,\boldsymbol{x}^N) \\ R(\boldsymbol{x}^2,\boldsymbol{x}^1) & R(\boldsymbol{x}^2,\boldsymbol{x}^2) & \text{[redacted]} & R(\boldsymbol{x}^1,\boldsymbol{x}^N) \\ \text{[redacted]} & & & \\ R(\boldsymbol{x}^N,\boldsymbol{x}^1) & R(\boldsymbol{x}^N,\boldsymbol{x}^2) & \text{[redacted]} & R(\boldsymbol{x}^N,\boldsymbol{x}^N) \end{bmatrix}. \tag{7}$$

The mean $\bar{\mu}_j$ is given by

$$\bar{\mu}_j = (\boldsymbol{1}^T\boldsymbol{R}^{-1}\boldsymbol{1})^{-1}\boldsymbol{1}^T\boldsymbol{R}^{-1}\boldsymbol{f}_j\,. \tag{8}$$

Correlation parameters θ_k are found by maximixing [4]

$$-[N\ln(\bar{\sigma}^2) + \ln|\boldsymbol{R}|]/2, \tag{9}$$

in which the variance

$$\bar{\sigma}_j^2 = (\boldsymbol{f}_j - \boldsymbol{1}\bar{\mu}_j)^T\boldsymbol{R}^{-1}(\boldsymbol{f}_j - \boldsymbol{1}\bar{\mu}_j)/N, \tag{10}$$

and $|\boldsymbol{R}|$ are both functions of θ_k.

D. Space Mapping Optimization Algorithm

The kriging coarse model is used to optimize the fine model using the standard space mapping algorithm of the form [3]:

$$\boldsymbol{x}^{(i+1)} = \arg\min_{\boldsymbol{x}} U\left(\boldsymbol{R}_s^{(i)}(\boldsymbol{x})\right), \tag{11}$$

where $\boldsymbol{x}^{(i)}$, $i = 0, 1, \ldots$ is a series of approximate solutions to (1) with $\boldsymbol{x}^{(0)}$ being the approximate optimum of the coarse-discretization model $\boldsymbol{R}_{cd}$ (cf. Section 3.*C*).

In this work, the kriging coarse model $\boldsymbol{R}_c$ is corrected using input and frequency SM [5] so that the SM surrogate model $\boldsymbol{R}_s^{(i)}$ is defined as:

$$\boldsymbol{R}_s^{(i)}(\boldsymbol{x}) = \boldsymbol{R}_s(\boldsymbol{x},[\boldsymbol{c}^{(i)}, f_1^{(i)}, f_2^{(i)}]) = \begin{bmatrix} R_c(\boldsymbol{x}+\boldsymbol{c}^{(i)}, f_1^{(i)} + f_2^{(i)}\omega_1) \\ \\ R_c(\boldsymbol{x}+\boldsymbol{c}^{(i)}, f_1^{(i)} + f_2^{(i)}\omega_m) \end{bmatrix}, \tag{12}$$

where

$$[\boldsymbol{c}^{(i)}, f_1^{(i)}, f_2^{(i)}] = \arg\min_{[\boldsymbol{c},f_1,f_2]} \sum_{k=0}^{i} \|\boldsymbol{R}_f(\boldsymbol{x}^{(k)}) - \boldsymbol{R}_s(\boldsymbol{x}^{(k)},[\boldsymbol{c},f_1,f_2])\|. \tag{13}$$

Using these simple SM transformations is normally sufficient because the kriging coarse model is built from the coarsely-discretized Sonnet model $\boldsymbol{R}_{cd}$ which is relatively accurate by itself.

3. Illustration Examples

A. Third-Order Chebyshev Bandpass Filter [23]

Consider the third-order Chebyshev bandpass filter [24 shown in Fig. 1. The design variables are $\boldsymbol{x} = [L_1\ L_2\ S_1\ S_2\ W_1\ W_2]^T$ mm. The fine model $\boldsymbol{R}_f$ is simulated in Sonnet ***em*** [13] using a grid of 0.1 mm ×

0.02 mm (evaluation time 15 min). The design specifications are $|S_{21}| \geq -1$ dB for 1.8 GHz $\leq \omega \leq$ 2.2 GHz, and $|S_{21}| \leq -20$ dB for 1.0 GHz $\leq \omega \leq$ 1.55GHz and 2.45 GHz $\leq \omega \leq$ 3.0 GHz. The initial design is $\boldsymbol{x}^{init} = [15\ 15\ 0.4\ 0.4\ 0.4\ 0.4]^T$ mm.

The coarse-discretization model $\boldsymbol{R}_{cd}$ uses a grid of 1.0 mm × 0.1 mm (evaluation time 55 s). Figure 2(a) shows the responses of $\boldsymbol{R}_{cd}$ at $\boldsymbol{x}^{init}$ and at $\boldsymbol{x}^{(0)} = [15\ 15\ 0.4\ 0.7\ 0.2\ 0.4]^T$ mm, its optimal design found using a pattern search. Figure 2(b) shows the responses of the fine model at $\boldsymbol{x}^{(0)}$ and at $\boldsymbol{x}^{(3)} = [15.3\ 18.8\ 0.44\ 0.72\ 0.14\ 0.34]^T$ mm (minimax specification error –0.41 dB), the optimal design obtained in three iterations of the SM algorithm using the kriging coarse model. The kriging model is set up using 80 evaluations of $\boldsymbol{R}_{cd}$. The optimization cost shown in Table 1 corresponds to 12 evaluations of the fine model.

B. High-Temperature Superconducting (HTS) Filter [24]

Consider the HTS filter shown in Fig. 3 [24]. The design parameters are $\boldsymbol{x} = [L_1\ L_2\ L_3\ S_1\ S_2\ S_3]^T$. The width of all the sections is $W = 8$ mil. A substrate of lanthanum aluminate is used with $\varepsilon_r = 23.425$ $H = 20$ mil. The filter is simulated in Sonnet ***em*** [13] using a grid of 0.5 mil × 0.5 mil (the $\boldsymbol{R}_f$ model). The design specifications are $|S_{21}| \leq 0.05$ for $\omega \leq 3.966$ GHz, $|S_{21}| \geq 0.95$ for 4.008 GHz $\leq \omega \leq$ 4.058 GHz, and $|S_{21}| \leq 0.05$ for $\omega \geq 4.100$ GHz. The initial design is $\boldsymbol{x}^{(0)} = [196\ 196\ 190\ 20\ 92\ 100]^T$ mil. The coarse-discretization model $\boldsymbol{R}_{cd}$ uses a grid of 2 mil × 4 mil. The evaluation times for $\boldsymbol{R}_{cd}$ and $\boldsymbol{R}_f$ are about 2 min and 51 min, respectively.

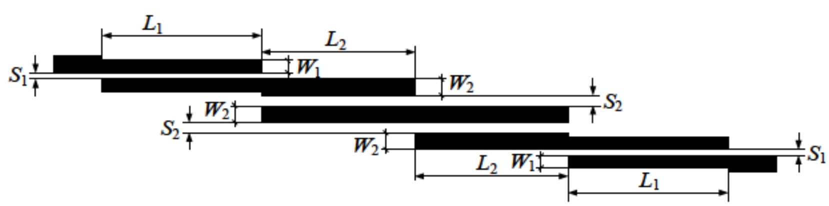

Fig. 1. Third-order Chebyshev bandpass filter: geometry [23].

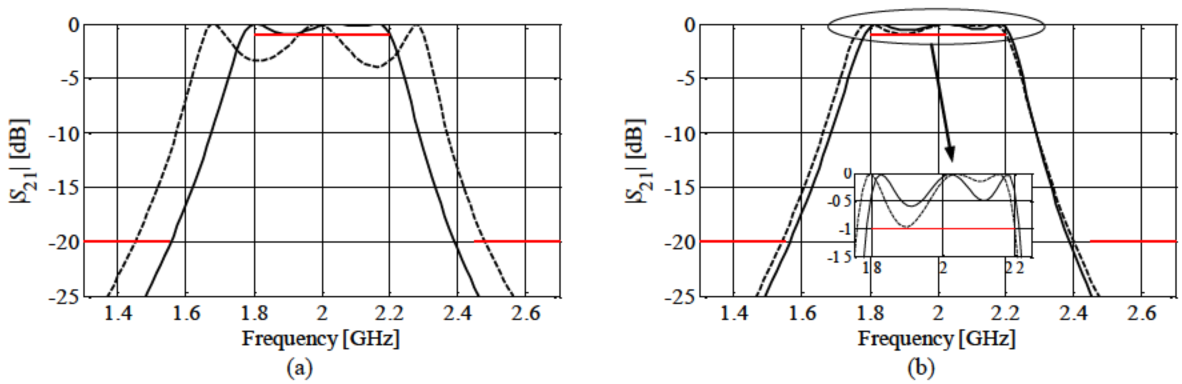

Fig. 2. Third-order Chebyshev bandpass filter: (a) responses of the coarse-discretization model $\boldsymbol{R}_{cd}$ at the initial design $\boldsymbol{x}^{init}$ (dashed line) and at its optimized design, $\boldsymbol{x}^{(0)}$, (solid line); (b) responses of the fine model $\boldsymbol{R}_f$ at $\boldsymbol{x}^{(0)}$ (dashed line) and at the final design $\boldsymbol{x}^{(3)}$ (solid line).

Table 1. Optimization cost of the third-order Chebyshev bandpass filter.

Algorithm Component	Number of Model Evaluations	Computational Cost	
		Absolute [min]	Relative to $\boldsymbol{R}_f$
Optimization of the coarse-discretization model $\boldsymbol{R}_{cd}$	$50 \times \boldsymbol{R}_{cd}$	46	3.1
Kriging coarse model setup	$80 \times \boldsymbol{R}_{cd}$	73	4.9
Evaluation of the original (fine-discretization) model $\boldsymbol{R}_f$	$3^* \times \boldsymbol{R}_f$	45	4.0
Total optimization time	N/A	164	12.0

* Excludes evaluation of $\boldsymbol{R}_f$ at the initial design

Figure 4(a) shows the responses of $\boldsymbol{R}_{cd}$ at $\boldsymbol{x}^{init}$ and at $\boldsymbol{x}^{(0)} = [188\ 190\ 188\ 20\ 76\ 84]^T$ mil, its optimal design found using a pattern search. Figure 4(b) shows the responses of the fine model at $\boldsymbol{x}^{(0)}$ and at $\boldsymbol{x}^{(2)} = [188\ 189.5\ 188\ 20\ 76\ 84.5]^T$ mil (minimax specification error –0.021), the optimal design obtained in one iteration of the SM algorithm using the kriging coarse model. The kriging model uses 50 evaluations of $\boldsymbol{R}_{cd}$. The optimization cost shown in Table 2 corresponds to about 7 evaluations of the fine model.

4. Conclusion

Simple and reliable procedure for microwave design optimization with Sonnet is proposed that utilizes coarse-discretization Sonnet simulations as the low-fidelity model of the structure under consideration. The low-fidelity model is used to obtain the initial approximation of the design and to create a fast coarse model for subsequent space mapping optimization of the original structure. The coarse model is created using kriging interpolation. Our technique is demonstrated through the design of two microstrip filters.

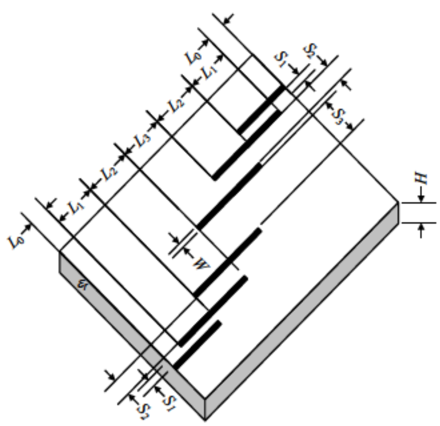

Fig. 3. HTS filter: geometry [24].

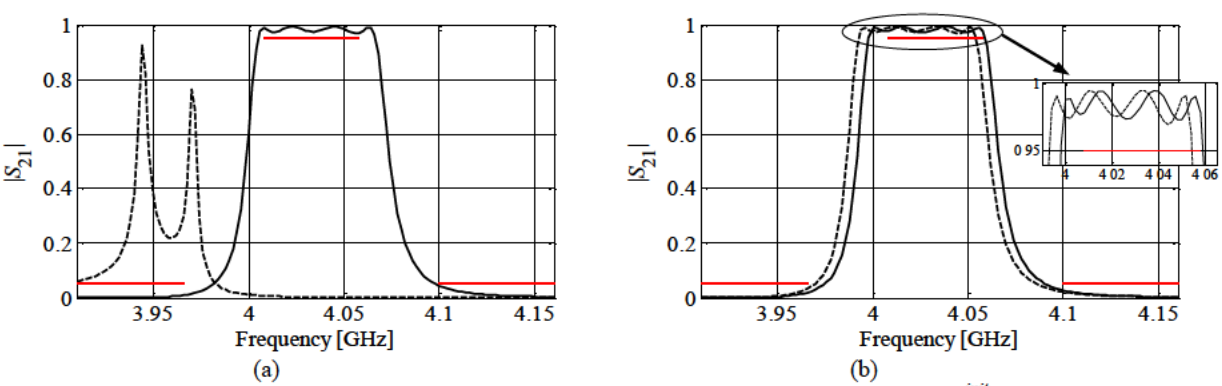

Fig. 5. HTS filter: (a) responses of the coarse-discretization model $\boldsymbol{R}_{cd}$ at the initial design $\boldsymbol{x}^{init}$ (dashed line) and at its optimized design, $\boldsymbol{x}^{(0)}$, (solid line); (b) responses of the fine model $\boldsymbol{R}_f$ at $\boldsymbol{x}^{(0)}$ (dashed line) and at the final design $\boldsymbol{x}^{(3)}$ (solid line).

Table 2. Optimization cost of the HTS filter.

Algorithm Component	Number of Model Evaluations	Computational Cost	
		Absolute [min]	Relative to $\boldsymbol{R}_f$
Optimization of the coarse-discretization model $\boldsymbol{R}_{cd}$	$100 \times \boldsymbol{R}_{cd}$	200	3.9
Kriging coarse model setup	$60 \times \boldsymbol{R}_{cd}$	120	2.4
Evaluation of the original (fine-discretization) model $\boldsymbol{R}_f$	$1^* \times \boldsymbol{R}_f$	51	1.0
Total optimization time	N/A	371	7.3

* Excludes evaluation of $\boldsymbol{R}_f$ at the initial design

Acknowledgement

The author thanks Sonnet Software, Inc., Syracuse, NY, for ***em***™. This work was supported in part by the Icelandic Centre for Research (RANNIS) Grant 110034021.

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