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ISBN 978-3-030-38925-3 ISBN 978-3-030-38926-0 (eBook)
https://doi.org/10.1007/978-3-030-38926-0

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

To our families: Dorota, Anna Halina,
Janusz, Kinga, Wladek, Bronek, and Stas

Preface

The development of modern high-frequency structures, including microwave and antenna components, heavily relies on full-wave electromagnetic (EM) simulation models. Notwithstanding, EM-driven design entails considerable computational expenses. This is especially troublesome when solving tasks that require massive EM analyses, parametric optimization, and uncertainty quantification being representative examples. The employment of fast replacement models, also referred to as surrogates, has been fostered as a way of mitigating these issues. Unfortunately, conventional modeling methods are of limited applicability for handling nonlinear outputs of high-frequency devices. The reason is the curse of dimensionality but also a fundamental requirement that design-ready surrogates are to cover wide ranges of the system parameters and its operating conditions. This book offers a different methodological perspective on modeling of high-frequency structures, specifically the concept and implementation of constrained or performance-driven surrogates. The presented approach addresses the issues of dimensionality and parameter ranges through appropriate confinement of the model domain, focused on the regions that are promising from the point of view of the relevant design objectives. The performance-driven paradigm enables the construction of reliable surrogates at a fraction of cost required by conventional methods and to accomplish modeling tasks where other techniques routinely fail. The book provides a broad selection of specific frameworks, extensively illustrated using examples of real-world microwave and antenna structures. Applications, including parametric optimization and multi-objective design, are also discussed, along with the exposition of inverse modeling methods. Furthermore, the book contains introductory material on data-driven and physics-based surrogates. Practical aspects of high-frequency surrogate modeling and recommendations concerning particular techniques are discussed as well.

Reykjavik, Iceland
Gdansk, Poland
December 2019

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Acknowledgments

We would like to acknowledge the efforts of all those students, researchers, and colleagues who have helped us during the research work presented in this book. We would also like to thank Dassault Systèmes, France, for making CST Microwave Studio available for our research purposes, Sonnet Software Inc. for Sonnet ***em***, and Keysight Technologies for ADS.

Contents

Chapter 1
Introduction

Computational models have become a backbone of contemporary engineering design. Their advantage over simpler (primarily analytical or semiempirical) methods of describing components and devices is in a capability of comprehensive handling and quantifying physical phenomena that affect the system operation, as well as in providing reliable values of performance figures pertinent to the design task being conducted. The development of computer hardware and simulation techniques has been unprecedented over the last several decades. Commercial simulation packages utilized in various fields, e.g., mechanical engineering (Fusion 360; Autodesk 2019), aerospace engineering (Inventor; Autodesk 2019), high-frequency electronics (Cadence Allegro 2019; Microwave Office, National Instruments 2019), multi-physics simulation (Multiphysics Simulation; ANSYS 2019; COMSOL Multiphysics, COMSOL Inc. 2018), etc., have reached a genuinely high level of sophistication. This is to the extent which makes it possible to evaluate complex structures and large-scale systems, e.g., antenna allocation on military vehicles (Byun et al. 2013), civil aircrafts (incorporating 3D model of the wings and the fuselage) (Liersch and Hepperle 2011), the ship on a random sea surface (Hao and Sheng 2017), or turbulent airflow through dual-rotor wind turbines (Rosenberg et al. 2014), as well as conduct multi-physics analysis (Keyes et al. 2013; Sharma and Sarris 2016; Cho et al. 2017; Fang et al. 2017; Szakmany et al. 2018; Ravelo 2018). Given reliable data on the material parameters and boundary conditions as well as sufficiently dense discretization of the structure at hand, the simulation models provide accuracy that allows us to replace costly prototyping.

In high-frequency electronics, the main application area of this book, the primary type of computational modeling is full-wave electromagnetic (EM) analysis (Davidson 2010; Sullivan 2013; Sevgi 2014; Swanson and Hoefer 2003; White 2004). By numerical solving of Maxwell equations established over a selected computational domain, it is possible to find the distribution of the electric and magnetic fields therein and, through appropriate post-processing, acquire relevant system characteristics such as scattering parameters (Nikolova et al. 2006) or radiation patterns (Paulotto et al. 2008). A large number of general purpose and specialized analysis

S. Koziel, A. Pietrenko-Dabrowska, *Performance-Driven Surrogate Modeling of High-Frequency Structures*, https://doi.org/10.1007/978-3-030-38926-0_1

techniques have been developed that are suitable for various purposes (e.g., finite-element analysis; Jin 2002; finite-difference time-domain analysis; Webb 2004; methods of moments; Gibson 2007, etc.). EM-driven design including design closure (in particular, adjustment of geometry and/or material parameters to fine-tune the system performance) has become an academic and industry standard. Nowadays, it is possible to conduct the entire design process within the simulation environment. Many commercial simulation software packages are available, including the general purpose EM solvers such as HFSS (HFSS 2019), Altair FEKO (FEKO 2018), CST Microwave Studio (CST 2018), XFDTD (XFDTD 2016), Momentum (Keysight 2019), or Sonnet *em* (Sonnet 2018), but also specific design tools (e.g., ADS; Advanced Design System, Keysight 2019, Antenna Magus; Antenna Magus 2019, for antenna design).

Initially, the main application of computational models was design verification. Rapid development of simulation techniques, software, and hardware, enabled a possibility of carrying out simulation-driven design. Undoubtedly, the most common design task is parametric optimization, where the values of selected variables are adjusted in order to improve the system performance (Bubnicki 2005; Zaslavski 2010; Pistikopoulos et al. 2007; Koziel and Bandler 2015; Koziel et al. 2016; Cao et al. 2011; Chakravorty and Mandal 2016; Sadrossadat et al. 2013). The latter is quantified by means of appropriately defined objective function (Koziel et al. 2013; Sobester and Forrester 2015). Other tasks include statistical design (e.g., Monte Carlo analysis; Styblinski and Opalski 1986) as well as uncertainty quantification (Hosder 2012; Allaire and Willcox 2014). A wide range of specialized algorithms have been developed to perform each of these tasks (Nocedal and Wright 2000; Conn et al. 2009; Gorissen et al. 2010; Yang 2010). Some of the methods are generic, i.e., applicable to a number of problems in different areas (Nocedal and Wright 2000); others are problem-specific (e.g., Koziel et al. 2013). It should be emphasized that utilization of the simulation models in the design processes has actually become a practical necessity for a growing number of components and systems. This is because traditional approaches, largely based on design-ready theoretical models, are no longer adequate. One of the reasons is the increasing level of complexity of engineering systems; another are various system- and component-level interactions that have to be taken into account in the design process (Kozakoff 2010; You et al. 2014; Bekasiewicz and Koziel 2015; Wang et al. 2018; Mandic et al. 2019).

Needless to say, simulation-driven design is quite a challenging problem for a majority of real-world cases. The fundamental issue is a high cost of evaluating the computational models. The simulation times very much depend on the model complexity and may be just a few seconds per frequency for simple electromagnetic (EM) analysis of two-dimensional models (e.g., planar microwave filters; Hazdra et al. 2005), a few minutes for computational fluid dynamics (CFD) analysis of two-dimensional airfoil profiles (Siegler et al. 2016) or EM analysis of compact planar antennas (Bekasiewicz and Koziel 2015), and up to a few hours (e.g., CFD analysis of three-dimensional structures such as aircraft wings, or EM analysis of integrated photonic components; Krause and Jäger 2005; Fakhfakh et al. 2015).

Particularly involved structures (a full aircraft, a ship, climate models) may require many hours or even days of the analysis time (Wehner et al. 2010; Dennis et al. 2012; Yondo et al. 2018). Interestingly, as the engineers consider more and more complex systems, the high-cost bottleneck is still there despite all the advancements in hardware and simulation software. Long analysis times can make simulation-driven optimization prohibitive when conventional algorithms are utilized as the latter typically require a large number of objective function evaluations. The problem is more pronounced for high-dimensional parameter spaces but also when global or multi-objective optimization is necessary. The most popular global search procedures involve population-based metaheuristics, which are extremely inefficient in computational terms (typical number of objective function evaluations ranges from a few thousands to many thousands per algorithm run). Another issue pertinent to computational models is the numerical noise, which may be a result of terminating the simulation process before full convergence, or it may be related to adaptive meshing employed by certain solvers. The latter manifests itself through noticeable changes of the simulated system responses due to even very small changes of the structure geometry (these leading to considerable changes of the mesh topology). The noise may affect the operation of gradient-based optimization routines that normally require the objective function to be smooth. The issues related to high cost of computational models can be mitigated to a certain extent by using adjoint sensitivities (Director and Rohrer 1969; Pironneau 1984; Jameson 1988; El Sabbagh et al. 2006; Papadimitriou and Giannakoglou 2008; Toivanen et al. 2009) or automated differentiation (Griewank 2000; Bischof et al. 2008). These methods allow for a fast evaluation of gradients of the figures of interest at small extra computational effort (often only one additional simulation) regardless of the number of designable parameters. Consequently, the benefits of adjoints are particularly evident for higher-dimensional problems. Adjoint sensitivities are currently available in some commercial simulation packages in various areas (e.g., computational fluid dynamics solvers: ANSYS Fluent 2015; Star-CCM+ 2015), as well as some noncommercial codes (e.g., Stanford University Unstructured; Palacios et al. 2013). In the context of high-frequency modeling, currently only CST Microwave Studio (CST 2018) and ANSYS HFSS (HFSS 2019) support this technology.

It should be mentioned that the challenges discussed in the previous paragraph led to the development of various interactive forms of utilizing simulation models in the design work, still commonly used in many areas. The key factor is the engineering insight, which allows for making reasonable predictions about the promising changes of the system parameters. The practical workflows typically involve parameter sweeping (usually, one parameter at a time). Experienced designers are often capable of identifying satisfactory parameter setups using an acceptable number of simulations even though the interactive procedures are rather laborious and do not guarantee optimum results. As a matter of fact, with the increasing complexity of the engineering systems, the efficiency of parameter sweeping has been declining, also because it is not able to handle multiple objectives and constraints.

Perhaps the most promising approach to handle expensive computer simulation is a utilization of fast replacement models, referred to as surrogates (Simpson et al.

2001; Queipo et al. 2005; Bandler et al. 2008; Forrester and Keane 2009; Koziel and Bekasiewicz 2016; Yondo et al. 2019). If a given system or device needs to be repeatedly evaluated, whether the purpose is parametric optimization, sensitivity analysis, yield estimation, or robust design, computationally cheap surrogate models become indispensable. Obviously, the computational burden can be relieved to a certain extent by using more efficient algorithms, e.g., those that exhibit faster convergence rates (in the context of numerical optimization). However, this is insufficient when thousands or tens of thousands of evaluations are required. For the surrogate to be effectively used instead of the original simulation model, it needs to be fast, sufficiently accurate, and, preferably, analytically tractable (e.g., smooth) (Alexandrov and Lewis 2001; Bandler et al. 2008; Jin 2011; Koziel and Leifsson 2013a). Depending on their application areas, the surrogates can be constructed locally (e.g., in the vicinity of the optimization path for the purpose of local optimization, or around the nominal design for the purpose of statistical analysis) or over the entire parameter space pertinent to a given problem (e.g., for the purpose of global optimization). Although surrogate models have been around for many decades, their importance has been steadily growing over the last two decades or so because of the increasing role of computational models themselves. The literature on surrogate models (also referred to as replacement models or metamodels; Simpson et al. 2001; Muller and Shoemaker 2014) is replete (Bilicz 2016; Declercq et al. 2013; Leary et al. 2003; Mendes et al. 2013; Du and Roblin 2018; Wang et al. 2018; Yang et al. 2019). This book is not an exposition of surrogate modeling in general but focuses on particular aspects of construction and application of replacement models in high-frequency electronics. Nevertheless, the necessary background material is included for the convenience of the reader. In particular, we provide a general classification of the surrogate models, highlight the stages of model construction and validation, as well as discuss a number of specific modeling methods. We also discuss various challenges and the ways of addressing them. More detailed outline of the book content is provided in the last paragraph of this chapter.

As explained before, surrogate modeling emerged from practical necessity: massive evaluations of the simulation models of certain kinds, especially those that require numerical solving of the systems of partial differential equations over large computational domains, were (and still are) unmanageable (Hazdra et al. 2005; Siegler et al. 2016; Bekasiewicz and Koziel 2015; Krause and Jäger 2005; Fakhfakh et al. 2015; Yondo et al. 2018). It should be made clear at this point that construction of the replacement models also requires quite a number of evaluation of the original model; however, the surrogate should ultimately ensure a reduction of the total computational overhead. This applies to both the library type of models for multiple use (e.g., models of individual components being building blocks of larger systems, Queipo et al. 2005) and the models constructed for a one-time use such as parametric optimization (De Tommasi et al. 2010). From that perspective, the appropriate selection of the modeling approach is an important yet a nontrivial task.

The surrogate modeling process consists of several steps. The first one is design of experiments, i.e., allocation of the training data set (Kleijnen 2018). Various sampling schemes have been developed, but, nowadays, the preferred approaches

are space-filling designs where the samples are allocated as uniformly as possible (Santner et al. 2018). The training data is then acquired at the selected points, and the surrogate model is identified according to the preferred modeling technique. In some cases, the model parameters may be found analytically; in others, a dedicated optimization process, often referred to as model training, has to be executed (Queipo et al. 2005; Bandler et al. 2008; Forrester and Keane 2009; Brigham and Aquino 2007). The final stage is model validation, where the quality of approximating the training data and/or generalization error (i.e., the ability of making predictions at the locations outside the training set) is estimated (Mack et al. 2007). The entire modeling cycle may be iterated by allocating additional training points according to specified rules (Kleijnen 2018) and re-identifying the model.

Despite a large variety of modeling techniques that can be found in the literature, two major types of the surrogates can be distinguished. The first type is so-called data-driven or approximation models, constructed from sampled high-fidelity simulation data (Simpson et al. 2001). The most popular techniques include polynomial regression (Jin et al. 2001), artificial neural networks (Haykin 1998), radial basis functions (RBF) (Wild et al. 2008), kriging (Jones 2001; Forrester and Keane 2009; Kleijnen 2009), support vector regression (Smola and Schölkopf 2004; Chávez-Hurtado and Rayas-Sánchez 2016), Gaussian process regression (Angiulli et al. 2007; Jacobs 2012), and multidimensional rational approximation (Shaker et al. 2009). The most important advantage of approximation models is their versatility. Because the surrogate is constructed merely using the data acquired from the system of interest, no physical insight is involved, and the mentioned techniques can be potentially applied to any type of problem. At the same time, data-driven surrogates are cheap to evaluate because they are essentially analytical models (e.g., linear combinations of appropriate basis functions in case of RBF; Rozhenko 2018). However, versatility comes at a price: in order to ensure the acceptable predictive power of the surrogate, the design space needs to be sampled with adequate density. As the modeling error mainly depends on the average distance between the training points and the nonlinearity of the system responses, one needs to ensure that the said distance is sufficiently small to capture the response changes across the model domain. This becomes the major bottleneck for approximation-based modeling because the average point-to-point distance scales poorly in high-dimensional spaces and large training data sets are necessary to construct usable surrogates (the effect also referred to as the curse of dimensionality; Wu et al. 2019). Depending on the functional landscape to be modeled, a typical number of training data samples ranges from a few hundred to many thousands. Construction of the surrogates within highly dimensional spaces (say, 20 or more dimensions) is only possible if the system responses are weakly nonlinear. In case of high-frequency electronics, practical data-driven modeling of components such as multiband antennas (characterized by sharp, resonant-like responses), filters (featuring multiple poles and transmission zeros), or compact microwave components (e.g., couplers), is limited to a few parameters. In the case of the mentioned structures, modeling within wide ranges of parameters is even more important for the surrogates to be of any utility for design purposes (Feng et al. 2019; Yelten et al. 2012; Koziel et al. 2013; Koziel and Bekasiewicz 2015;

Koziel et al. 2016). This poses even more challenges than the dimensionality issue because characteristic features of the responses (e.g., the resonances) change considerably along the frequency spectrum (Koziel and Bekasiewicz 2017a; Koziel and Bekasiewicz 2017b; Koziel and Bekasiewicz 2018a; Koziel and Bekasiewicz 2018b; Ullah and Koziel 2019; Rossi et al. 2014). Consequently, in practice, globally accurate approximation modeling is usually justified in case of multiple-use library models of components described by a limited number of parameters. Overcoming these issues is one of the main topics of this book.

It should be mentioned that global data-driven modeling—mostly for the purpose of design optimization—has been nowadays dominated by the surrogates iteratively improved through sequential sampling (Couckuyt et al. 2012). Various ways of incorporating new training points into the model (so-called infill criteria) have been developed, including exploitative models (i.e., models oriented toward improving the design in the vicinity of the current one), explorative models (i.e., models aiming at improving global accuracy), as well as model with balanced exploration and exploitation (Forrester and Keane 2009; Couckuyt et al. 2010). Generally, these techniques are often referred to as efficient global optimization (EGO) methods (Jones et al. 1998) or surrogate-assisted evolutionary algorithms (SAEAs) (Gorissen et al. 2009; Lim et al. 2010; Jin 2011; Yang et al. 2019).

The second major class of surrogates is physics-based models. The term "physics-based" relates to the fundamental structure of these surrogates which exploit, to a certain extent, the system-specific knowledge (Cervantes-González et al. 2016; Koziel and Leifsson 2016). This, in turn, is most often some sort of simplified physical description of the system in the form of an underlying low-fidelity model (Robinson et al. 2008; Koziel and Leifsson 2013b; Sarkar et al. 2019). The low-fidelity model is subsequently corrected using a limited amount of high-fidelity simulation data, typically through linear or nonlinear regression (Bandler et al. 2004). A representative example of a low-fidelity model in the area of microwave engineering is an equivalent network of the structure (e.g., a filter), with the high-fidelity model being evaluated through a full-wave electromagnetic analysis (Zhu 2002). Clearly, the equivalent network based on the circuit theory rules does not ensure accuracy comparable to the full-wave simulation involving numerical solutions to Maxwell's equations, e.g., it does not account for the cross-coupling effects within the structure, but it is definitely faster. The fundamental benefit of this type of arrangement is that due to the same physics shared by the low- and high-fidelity models, the surrogate is likely to exhibit a better generalization capability, it is valid over wider ranges of parameters, and it is less prone to suffer from the curse of dimensionality. At the same time, the number of high-fidelity training samples is substantially smaller than required by the approximation models. In other words, physics-based modeling solves some of the issues of data-driven surrogates, which has been the primary reason for its growing popularity (Pantoja et al. 2007; Salleh et al. 2008; Crevecoeur et al. 2010; Koziel and Leifsson 2013a; Cervantes-González et al. 2016; Koziel et al. 2016; Baratta et al. 2018; Zhang et al. 2018). Unfortunately, the same factors that contribute to the attractiveness of the physics-based surrogates also imply their limitations. The first issue is the low-fidelity model itself. It is

normally problem-specific (Bandler et al. 2004; Koziel and Leifsson 2013a); therefore, physics-based surrogates lack versatility of the data-driven models. Low-fidelity models can be obtained in various ways: (i) as analytical models (in practice, a set of design-ready equations offering a considerably simplified description of the system; Koziel et al. 2014), (ii) by simulating the system at a different level (e.g., in microwave engineering: equivalent circuit representation evaluated using circuit theory rules versus full-wave electromagnetic simulation; Bandler et al. 2004), and (iii) lower-fidelity or lower-resolution simulation (e.g., simulation with coarser discretization of the structure and/or relaxed convergence criteria; Koziel and Ogurtsov 2014). Because the low-fidelity models typically involve computer simulation, their evaluation time cannot—in many cases—be neglected, and the aggregated computational cost of the low-fidelity model simulation may be significant in certain applications, e.g., parametric optimization (Zhou et al. 2007; Koziel and Leifsson 2016). Another issue is a trade-off between the low-fidelity model speed and accuracy. While this can be easily adjusted in many situations, e.g., by changing the discretization density in coarse-mesh simulation models (Koziel and Bekasiewicz 2016), selection of a particular model setup might not be a trivial task (Koziel and Ogurtsov 2012).

Surrogate models are finding applications wherever reduction of the computational overhead due to massive evaluations of the computational model is of concern. Probably the most popular application area is design optimization (Booker et al. 1999; Bandler et al. 2004; Queipo et al. 2005; Forrester and Keane 2009; Koziel et al. 2011; Sóbester et al. 2012; Tabatabaei et al. 2015). Similarly, in high-frequency electronics, surrogate models are widely used for optimization purposes (Koziel and Leifsson 2013a; Lim et al. 2015; Lourenço and Lebensztajn 2015; Koziel et al. 2016; Koziel and Bekasiewicz 2016; Rangel-Patiño et al. 2017; Bramerdorfer and Zăvoianu 2017; Feng et al. 2019). Surrogate-based optimization (SBO) replaces direct optimization of the expensive high-fidelity model in the form of an iterative prediction-correction scheme, in which the surrogate guides the optimization process toward a better design, and it is subsequently refined using the high-fidelity data acquired along the way (Forrester and Keane 2009; Koziel and Leifsson 2013a). Because most of the operations are executed on the surrogate, the overall cost of the optimization process can be greatly reduced as compared to direct handling of the high-fidelity model (Koziel and Leifsson 2013a; Koziel and Ogurtsov 2014; Koziel and Bekasiewicz 2016). The SBO algorithms may be local ones (Zhou et al. 2007), with the surrogate constructed along the optimization path, or global (Iuliano and Andrés Pérez, (Iuliano and Andrés 2016)), where the model is constructed within a larger portion or the entire parameter space pertinent to the problem at hand. A simple example of the former is sequential approximate optimization (SAO), usually employing simple polynomial type of surrogates established within the domain that is relocated upon fining new and better designs (Kitayama et al. 2011). Global methods often follow the concept of the efficient global optimization (EGO) mentioned earlier in this chapter (Jones et al. 1998).

Physics-based surrogates are typically used for a local optimization. One of the most popular physics-based SBO methods in high-frequency electronics is space

mapping (SM) (Bandler et al. 2004; Koziel et al. 2008) which comes in many variations (aggressive SM, Bandler et al. 1995; implicit SM, Koziel et al. 2011; manifold mapping, Echeverria et al. 2006; neural SM, Gutiérrez-Ayala and Rayas-Sánchez 2010; output SM, Ayed et al. 2012; input SM, Khalatpour et al. 2011). For an overview of the methods that emerged from space mapping, the reader is directed, e.g., to Rayas-Sanchez (2016). Because the most straightforward way of constructing the surrogate model from the underlying low-fidelity model is correcting its response, many physics-based SBO algorithms employ such mechanisms. Some of the techniques include approximation model management optimization (AMMO; Alexandrov and Lewis 2001), multipoint correction (Toropov 1989), manifold mapping (Echeverria and Hemker 2005), adaptive response correction (Koziel et al. 2009), shape-preserving response prediction (Koziel 2010), or adaptive response scaling (Koziel and Unnsteinsson 2018). Apart from design optimization, surrogate models are used for many other purposes as well. An important area is uncertainty quantification (e.g., yield estimation; Bandler et al. 2002; Biernacki et al. 2012) and tolerance-aware (or robust) design (Ko et al. 2011; Koziel and Bandler 2015; Kouassi et al. 2016; Aubry et al. 2016). Statistical analysis is typically performed in order to find the effects of manufacturing tolerances or uncertainties concerning operating conditions on the system performance. Traditional methods such as Monte Carlo (MC) simulation (Hu et al. 2016, Liu 2017) are computationally heavy, and fast surrogates seem to be an ideal way of accelerating the process. Certain types of models, such as polynomial chaos expansion (PCE), are particularly suitable in this context due to their capability of directly assessing the statistical moments of the output probability distributions without the necessity of running MC (Sudret 2008; Xiu 2009; Du and Roblin 2017; Manfredi et al. 2017). Another important application of surrogates is inverse modeling which allows us to directly yield the optimum values of design variables corresponding to the required values of performance figures (Akkaram et al. 2007; Kabir et al. 2008; Koziel et al. 2016; Liu et al. 2016; Zhang et al. 2018).

The unquestionable benefits of using surrogates as a way to alleviate the difficulties related to massive evaluation of expensive simulation models should not overshadow the practical problems related to surrogate model construction. As already mentioned, the fundamental issue is the curse of dimensionality, or, more generally, extremely disadvantageous relations between the predictive power of the surrogate, the size of the parameter space—that depending on both its dimensionality and the parameter ranges—and the number of training samples. Nonlinearity of the system responses to be modeled (as functions of designable parameters) only make the situation more complex. There have been many attempts and techniques developed to mitigate these problems. One of them is sequential sampling (Xiong et al. 2009; Mukhopadhyay 2011; Wei et al. 2012; Mackman et al. 2013; Xu et al. 2014), nowadays commonly used as a design of experiments approach for data-driven surrogates. The idea is to replace a one-shot (typically uniform) sample allocation by an iterative process in which additional (or infill) samples are distributed based on the feedback obtained from the current sample distribution and/or the current surrogate. In the case of explorative design of experiments schemes (Mandal

et al. 2012), the infill samples are added without referring to the system output but merely based on the data points allocated so far, with the purpose of improving uniformity of the set. In general, especially for the exploitative sampling schemes (Koziel and Ogurtsov 2019), a suitable infill criterion may be maximization of the mean square error, i.e., identifying locations where the error (as predicted by the surrogate, typically, kriging) is the highest (Jiang et al. 2018). In these cases, finding infill points requires global optimization, typically realized using population-based metaheuristics (Beheshti and Shamsuddin 2013; Mehmani et al. 2015; Park et al. 2018; Liu et al. 2018), which makes the procedure slow. The advantage is that more samples may be allocated in the regions corresponding to higher nonlinearity of the system responses, which improved the model accuracy. Unfortunately, this sort of approach rarely pays off for many high-frequency structures where "nonlinear" regions are almost everywhere within the model domain (San et al. 2004; Hajjaj et al. 2017; Shitvov et al. 2014). Co-kriging (Forrester et al. 2007) and gradient kriging (Han et al. 2013) are other ways of reducing the computational cost of the training data acquisition. Co-kriging uses densely sampled low-fidelity model data blended together with a limited number of high-fidelity points which allows for constructing the surrogate of the accuracy similar to that obtained solely from (densely sampled) high-fidelity simulations. This is of course under the assumption that the low- and high-fidelity models are sufficiently well correlated. Gradient kriging, on the other hand, incorporates sensitivity data into the surrogate, which also potentially reduces the number of necessary training points; however, this approach is only practical if the gradient information can be obtained in a computationally efficient matter (e.g., through adjoints; Giles and Pierce 2000; Allaire 2015).

A different approach to handle dimensionality issues is high-dimensional model representation (HDMR) (Foo and Karniadakis 2010; Ma and Zabaras 2010; Shan and Wang 2011a; Cai et al. 2017; Liu et al. 2018; Wu et al. 2019), where the system responses are represented as a linear combination of functions that account for lower-order effects, specifically cooperative effects of single variables, pairs of variables, etc. Because domain dimensionalities of the functions contributing to the aforementioned expansion are low as compared to that of the original parameter space, considerable savings can be achieved in terms of the training data acquisition assuming that the higher-order interactions are weak and the corresponding expansion terms can be neglected (Shan and Wang 2011b). Clearly, HDMR is only applicable to systems that satisfy this assumption, which is, unfortunately, not the case for many high-frequency structures for that matter. Model order reduction (MOR) is another class of methods that generally refers to various ways of reducing the complexity of large-scale dynamical systems, while preserving (as much as possible) their input-output behavior (Baur et al. 2014; Henneron and Clénet 2014). The reduced models mimic (from the point of view of the input and output) the behavior of the large-scale system so that they can be efficiently used for design automation, parametric optimization, or sensitivity analysis. Particular numerical techniques utilized by MOR include, among others, Krylov subspace methods (Lin et al. 2007), Proper Orthogonal Decomposition (POD; Wilcox and Peraire, 2002),

principal component analysis (PCA; Dray 2008), solution space projection (SSP; Lee and Jin 2007), or rational approximation (Deschrijver et al. 2007). Examples of MOR in high-frequency engineering include parameterized MOR models of complex electromagnetic systems (Burgard et al. 2013; Sato et al. 2015), reduced order macromodels of high-speed microstrip structures (Zhu and Cangellaris 2001), and accelerated frequency sweeps in FEM analysis (de la Rubia et al. 2009). Several methods have also been developed to handle situations when the regression problem (e.g., in construction of response surface approximation models; Khuri and Mukhopadhyay 2010) is heavily underdetermined. This essentially means that the system at hand is characterized by a large number of internal degrees of freedom (e.g., analog or mixed-signal circuits, analog-to-digital converters, or RF front ends), whereas the regression model has to be built using a relatively small number of samples due to the computational budget issues or simply numerical problems pertinent to handling large data sets. Orthogonal matching pursuit (Tropp 2004; Tao et al. 2016; Li 2010; Bishop 2006) is a technique that identifies a small set of basis functions that approximate the model (or function) of interest. In order to ensure fast convergence, a set of basis functions that are normalized and orthogonal is normally adopted (Needell and Tropp 2009). Another method, Bayesian model fusion (Wang et al. 2013; Wang et al. 2016), can be classified as a physics-based surrogate technique because it uses the so-called early-stage data (e.g., schematic-level simulation data) in order to fit the late-stage model (e.g., a post-layout one with extracted parasitic components) (Li et al. 2012). By blending these two-level data, realized using Bayesian inference, the overall cost of model construction can be greatly reduced because very few late-stage samples are typically used (Tao et al. 2019).

The primary purpose of this book is a discussion of surrogate modeling techniques oriented toward simulation-based design optimization of high-frequency structures. The typical problems encountered here include vector-valued and highly nonlinear responses of the components and systems, multiple performance figures that have to be controlled, medium- to high-dimensional parameter spaces, as well as wide ranges of the parameters. For these types of problems, conventional surrogate modeling methods are insufficient. The book describes a number of methods, referred to as performance-driven modeling, that offer a way of overcoming the aforementioned difficulties. We discuss both forward and inverse models as well as how to apply them for rapid design purposes. The main theme is a utilization of an a priori prepared set of reference designs optimized for the selected values of performance figures of interest and defining the surrogate model domain based on this data (Koziel 2017; Koziel and Bekasiewicz 2017a; Koziel and Sigurðsson 2018; Koziel et al. 2018). This approach permits a dramatic reduction of the parameter space region that need to be sampled for the purpose of a model construction without formally reducing the parameter ranges (Koziel et al. 2019; Koziel and Pietrenko-Dabrowska 2019a; Koziel and Pietrenko-Dabrowska 2019b). In order to be self-contained, the book also contains some background material concerning both the data-driven and physics-based surrogate modeling. The material is organized in the following manner. Chapter 2 provides an overview of the surrogate modeling

process, including design of experiments, model identification and validation, as well as discusses a number of popular data-driven modeling methods. Chapter 3 introduces the concept and implementation of physics-based modeling. Chapters 4, 5, 6, 7, 8, and 9 contain exposition of performance-driven modeling approaches, including, among others, triangulation-based constrained modeling, nested kriging modeling, feature-based constrained modeling, as well as variable-fidelity modeling. Chapters 10 and 11 discuss application of performance-driven modeling for multi-objective design optimization as well as expedited (warm-start) optimization, respectively. Chapter 12 outlines various physics-based surrogate modeling techniques involving response correction, whereas Chap. 13 focuses on utilization of inverse surrogates for accelerated simulation-driven design of high-frequency structures. Chapter 14 concludes the work. The book is illustrated with a large number of practical design cases from various areas of high-frequency electronics, especially microwave and antenna engineering. Despite this particular focus, most of the modeling methods discussed here are of a generic nature and can be applied to a variety of problems in other engineering disciplines. The authors believe that the presented material may be helpful for engineers and researchers interested in applying surrogate modeling techniques in their design work, especially while solving tasks such as design optimization or for other projects that require massive evaluations of expensive computer simulation models.

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