AN EFFICIENT DESIGN OPTIMIZATION FRAMEWORK FOR RF AND OPTICAL APPLICATIONS

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ABSTRACT

Metamaterials have gained considerable interest in the RF and optics community due to their unusual properties not available in nature. However, despite their proven potential in theory and some practical realizations, metamaterials are restricted to some known geometry or physical compositions such as the SRR structure. This is largely due to the natural limit imposed by intuitive design efforts and or practical realization challenges. A formal efficient framework allowing for the design of non-intuitive structures does not exist. Similar to metamaterials, artificial composite designs in literature prompt for the possibility of unique material combinations possibly in three dimensions leading to desired electromagnetic behavior such as non-reciprocality. Formal design optimization can explore unknown design degrees of freedom. However, large scale design optimization problems such as volumetric material explorations are computationally very expensive and demand high resources. This drawback can be surpassed by introducing surrogate modeling techniques into the platform as demonstrated in literature. To address this issue, in this thesis, we present an efficient design optimization framework for electromagnetic applications. The framework is based on integrating design optimization techniques with various surrogate modeling tools. The goal is to identify the device structure, both material and conductor in three dimensions, in an automated and efficient manner subject to some performance and size constraints. For the synthesis module, gradient-based optimizers such as Sequential Quadratic Programming (SQP) and global optimizers such as Genetic Algorithms are both utilized. As the analysis module, full wave electromagnetic wave analyzers, such as the HFSS, and a hybrid FE-BI based electromagnetic solver (FSDA) are integrated to the optimizers. The design framework is primarily based on interfacing the analysis tools with various surrogate based models and linking it to the chosen optimization tool. The proposed

framework is modular, hence allows for various combinations of synthesis and analysis modules within different surrogate based models.

To allow for considerable speed-ups of the automated design process proposed here, automated and adaptive Design of Experiment (DOE) scheme is employed and various surrogate models are compared within the design framework with respect to their performance. Multiple surrogate modeling techniques are investigated such as Kriging, Polynomial, RBF (Radial Basis Functions), Artificial Neural Networks (ANN), Support Vector Machines (SVM), etc. Results suggest that the ANN surrogate model based design framework allows for large number of design variables and an effective exploration of the global large scale design space while RBF, SVM and Kriging are also successful at capturing resonance behavior. Multi-objective optimization method called Normal-Boundary Intersection (NBI) is integrated our framework. The resulting framework is suitable for the design of volumetric material compositions of applications such as an ultra-wide bandwidth SATCOM antenna and plasmonic nano-antennas. Future work comprises the determination of the artificial material structure following a two step procedure: The effective medium of the antenna is to be determined using the proposed surrogate based design optimization framework. This should allow for extending the capabilities of the proposed framework to the design of the microstructure of metamaterials utilizing inverse topology optimization. The freedom to explore all possible design degrees of freedom and the possibility to design for the material itself are expected to open up entirely new breakthroughs in microwave and optical applications.

RF ve Optik Uygulamalara Yönelik Hızlı Bir Tasarım Optimizasyon Sistemi

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Anahtar Kelimeler: Tasarım optimizasyonu, metamalzemeler, vekil modeller, meta modeller, mikro şerit antenler, nano antenler, genetic algoritmalar, yapay sinir ağları

Metamalzemeler doğa ötesi sergiledikeri özellikleriyle, RF ve optik çevrelerde büyük ilgi uyandırmıştır. Ancak, teoride ve bazı pratik uygulamalardaki potansiyeline rağmen metamalzemeler sadece SRR yapıları gibi bazı geometri ve kompozitlerle sınırlı kalmıştır. Bunun sebebi büyük ölçüde sezgisel tasarım çabalarının yetersizliği ve pratik olarak gerçekleştirilmelerindeki güçlüklerdir. Düşünmeyle bulunamayacak derecede kompleks yapıların tasarlanmasına izin verecek formal ve etkili bir sistem bulunmamaktadır. Literatürde yapay kompozit tasarımlar da metamalzemelere benzer olarak istenen elektromanyetik davranışı sergileyecek (örneğin non-reciprocality) eşsiz malzeme kombinasyonlarının varlığı olasılığını kuvvetlendiriyorlar. Formal Tasarım Optimizasyonu, bilinmeyen dizayn serbestlik derecelerini keşfedebilir. Ancak hacimsel malzeme belirlerme gibi büyük ölçekli tasarım optimizasyonu problemleri yüksek işlemci zamanı gerektirmektedirler. Bu darboğaz, literatürde belirtildiği gibi tasarım optimizasyonu sistemine vekil modelleme tekniklerinin entegre edilmesiyle aşılabilir. Bu problemi çözmek amacıyla, bu tezde elektromanyetik uygulamalar için hızlı bir tasarım optimizasyonu sistemi geliştirilmiştir.

Sistem, tasarım optimizasyonu tekniklerinin, çeşitli vekil modelleme yöntemlerinin birleştirilmesiyle gerçekleşir. Amacımız, tasarlanan cihazın yapısını, üç boyutta malzeme ve iletken dağılımını, otomatik ve etkili bir şekilde, bazı performans ve boyut kriterlerine sadık kalarak bulmaktır. Sentez modülü olarak, türev tabanlı optimizasyon algoritmaları, örneğin Sequential Quadratic Programming (SQP), ve global optimizsyon algoritmaları, örneğin Genetik Algoritmalar, kullanılmıştır. Analiz modülü olarak da tam dalga elektromanyetik dalga analizörü, HFSS ve hibrit sonlu eleman-sınır integrali metoduna dayanan elektromanyetik çözümleyici (FSDA), optimizasyon algoritmalarına entegre edilmiştir.

Tasarım sistemi öncelikli olarak analiz modülü ile çeşitli vekil modellerin arayüzlerinin oluşturulması, sonrasında da bu arayüzlerin seçilen optimizasyon algoritmasıyla birleştirilmesine dayanır. Önerilen sistem modüler olup, çeşitli sentez ve analiz modüllerinin farklı vekil sistemlerle çalışmasına izin verir.

Bu çalışmada önerilen, otomatik tasarım sisteminde önemli derecede hızlandırmayı mümkün kılmak için, otomatik ve adaptif deney tasarımları oluşturulmuş ve çeşitli vekil modeller, tasarım optimizasyonu sisteminde, performanslarına göre değerlendirilmiştir. ANN, RBF, SVM, Kriging, Rational gibi çeşitli vekil modelleme yöntemleri incelenmiştir. Sonuçlar göstermektedir ki ANN vekil modeliyle çalışan tasarım optimizasyonu çok sayıda tasarım değişkeninin incelenmesine ve global yüksek ölçekteki tasarım uzayının keşfine izin vermektedir. Ayrıca RBF, SVM ve Kriging metotları da ANN kadar olmasa da resonans davranışını modellemede başarılıdırlar. Çok amaçlı optimizsayon methodu Normal-Sınır Kesişimi (NBI), tasarım optimizasyonu sistememize entegre edilmiştir. Ortaya çıkan sistem, hacimsel malzeme komposizyonlarıyla yapılan ultra geniş bandgenişliğine sahip SATCOM antenlerinin ve plasmonik nano antenlerin tasarımına uygundur. Gelecekteki çalışmalarımızda, yapay malzemenin yapısı iki adımda belirlenecektir: Öncelikle önerilen vekil tabanlı tasarım optimizyonu sistemi kullanılarak antenin efektif malzemesi bulunacaktır. Böylece, metamalzemenin mikroyapısının ters-homojenizasyon ile belirlenmesini sağlayacak düzeye kadar önerilen sistemin yeteneklerinin geliştirilmesine izin verilecektir. Tüm tasarım değişkenlerini keşfetme özgürlüğü ve malzeme için tasarım yapabilme olasılığının kendisi bile mikrodalga ve optik uygulamalar için çığır açacak gelişmelere gebedir.

To my father and mother

and also,

“To the metamorphosis of us before flying through the valleys of life and our never ending search for the highest and sometimes the lowest hills for the sweetest flowers”

– Orkun KARABASOGLU

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ABBREVIATIONS

ANN	Artificial Neural Network
BLUP	Best Linear Unbiased Predictor
DACE	Design and Analysis of Computer Experiments
EM	Electro-magnetics
FSDA	Fast Spectral Domain AlgorithmGA Genetic Algorithms
HFSS	High Frequency Structure Simulator
IID	Independent and Identically Distributed
PBG	Photonic Band Gap
RBF	Radial Basis Functions
RRSE	Root Relative Square Error
SQP	Sequential Quadratic Programming
SUMO	Surrogate Modeling Toolbox SVM Support Vector Machines

1 INTRODUCTION

1.1 Engineered Novel Materials

"Engineers are starting to play God a bit.
We have been able to invent and implement novel materials
and devices where we tell the materials
how to behave."
—Federico CAPASSO

Engineered materials, such as metamaterials, new composites, electromagnetic bandgap, and periodic structures [1] have attracted considerable interest in recent years due to their remarkable and unique electromagnetic behavior. These new materials shown in Fig 1.1 may lead to the development of novel devices such as miniature antennas with high bandwidth and gain, optical antennas with superior properties, a perfect lens, capable of imaging objects with resolution much smaller than the wavelength of light, ultra-compact optical circuits, and cloaking devices leading to invisibility.

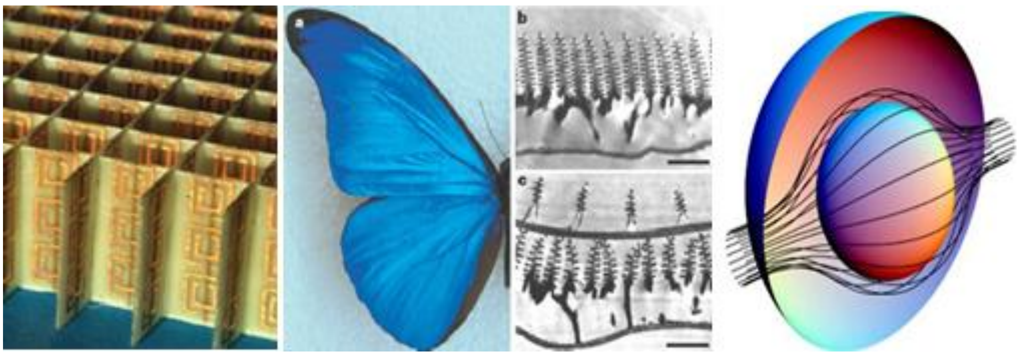

Fig. 1.1. Metamaterial, PBG in nature, Cloaking (From left to Right) [73-75]

As a result, an extensive literature on the theory and application of artificially modified materials exists. Already photonic crystals have been utilized in RF applications due to their extraordinary propagation characteristics [2], [3]. More recently, computations using double-negative materials [4], [5] and photonic crystals [6] illustrate that extraordinary gain can be achieved when small dipoles are placed inside other exotic materials that exhibit resonance at specific frequencies. Of importance is that recent investigations of material loading demonstrate that substantial improvements in antenna performance can be attained by loading bulk materials such as ferrites or by simply grading the material subject to specific design objectives [7].

Ceramics with multitone materials have also been used for miniaturization [8] and pliable polymers [9] possibly with ceramics or ferrite power loading offer new possibilities in three dimensional (3D) volumetric antenna design and multilayer printed structures, including 3D electronics. Metamaterials are used for variable bandwidth EM devices, electrically small resonant antennas, novel antennas and lenses [10].

Among the most exciting new applications for 3D low-loss metamaterials are those based on transformation optics [11], [12] and [13], including hyper-lenses that enable sub-wavelength far-field resolution [14], and designs for optical cloaking [15]

1.2 Design Optimization

Despite the novelty that new materials are promising, there are challenges and limitations when it comes to their design and practical realization. However, sophistication in formal design and fabrication techniques has allowed a major change in the way that these materials are realized. Using a computational model integrated with mathematical optimization techniques, many design candidates can be evaluated in a fraction of time required by real world experiments. Optimization is the science of finding the best and it has found many applications by finding good solutions to real world problems. However, many of these efforts assume that the objective function can be expressed algebraically and in explicit form. This means that the evaluation of the function is quick when a new set of variables is introduced. Furthermore, it is often necessary to differentiate the function, which guides algorithms towards the local optimum. However, most of the time engineering designs are so complex that their performance can only be evaluated by running a computational model. Most of the time, this model is created by numerical methods for finding approximate solutions of partial differential equations (PDE) as well as integral equations such as a finite element model. As new design variables are introduced to the synthesis module which basically consists of an appropriate optimization algorithm, it is necessary to run the model at each iteration of the design cycle. Furthermore, if the optimizer is a local technique relying on gradients of the objective function, these are most of the time to be calculated using finite difference approximations. Therefore, the bottleneck of almost all design optimization efforts is the cost associated with running the computational model repetitive times.

1.3 Surrogate Modeling

Large scale design optimization problems such as volumetric material explorations are computationally very expensive and demand high resources. One way of surpassing this drawback is by introducing surrogate modeling techniques into the platform as has been demonstrated in literature. Surrogate models are fast-running approximate substitutes of complex and time-consuming computer simulations of the exact model. Surrogate models are also known as response surface models (RSM), metamodels or emulators. They mimic the complex behavior of the underlying simulation model and they are model specific.

The principal motivation behind using surrogate models is associated with the prohibitive computational cost in running simulations for a large number of times during an iterative design cycle [16]. One model evaluation may take many minutes, hours, days or even weeks [17]. Nevertheless, one could argue that in order to obtain an accurate global surrogate one still needs to perform numerous simulations, thus running into the same problem. However, this is not the case since: (1) building a global surrogate is a one-time, up-front investment (assuming the problem stays the same), (2) distributed computing can speed-up the evaluation time, and (3) adaptive modeling and adaptive sampling (sequential design) can drastically decrease the required number of data points to produce a good model [18]. Hence, the goal in this thesis is to investigate surrogate based models comparatively for the material based design of electromagnetic devices, such as antennas.

1.4 Previous Work

1.4.1 Design Optimization for EM Design

Over the recent years, there has been strong interest in design optimization for electromagnetic (EM) applications [19]–[22]. These studies include mostly size and shape optimization rather than material optimization. Shape optimization is more common than size optimization, however, volumetric design would provide for greater design possibility. To take full advantage of volumetric variations in EM design we need an optimization framework that can simultaneously choose the best geometric and topological configuration while taking into consideration geometry as well as material composition. Such methods are called topology optimizations. It is reasonable to expect that designs resulting from topology optimization have novel configurations with higher performance as compared with designs resulting by size and shape optimizations as demonstrated in [23], [31] Since the paper by Bendsoe and Kikuchi in 1988 [24], topology optimization has expanded, successfully being applied to many practical engineering problems [25], [26]. This method has been widely accepted in industry/university as a potential design tool [27]. In EM, there have been various studies on the topology optimization of electrical devices [28], [29]. These have primarily dealt with problem-specific or semi-analytic tools for magneto-static applications. Recent formulations of topology design optimization problems allows for creating novel configurations through the integration of design optimization tools with robust finite element-boundary integral (FE-BI) [30] methods suitable for general EM problems [31-32]. The latter removes limitations on geometry and material distribution and also it incorporates fast O(N) solvers for rapid solution of large scale design problems. The general framework is given in Fig. 1.2. Accurate results employing the simulator have already been obtained for scattering and radiation by cavities, slots, and multilayer patch antennas and frequency selective surfaces, demonstrating the method’s capability. However, these studies have been both limited to local optimization techniques and dielectric material variation only or global design search studies with restricted design space such as few material design blocks within symmetric material distributions.

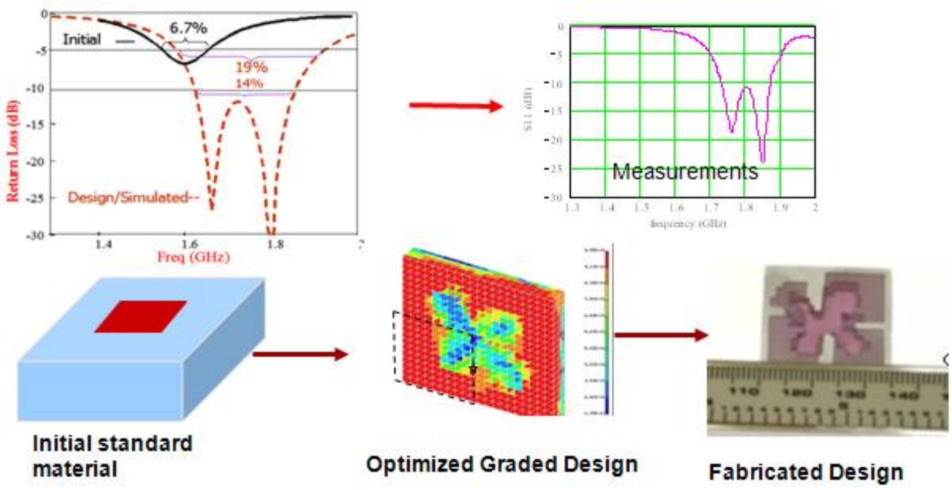

Fig. 1.2 Previous successes in topology optimization [23].

1.4.2 Surrogate Modeling

Numerical simulation and analysis is used extensively in electromagnetics community for design of new devices. Despite the never ending growth of computing power and technology, the computational cost of complex high-fidelity engineering analyses and simulations maintains pace. There have been recent attempts to deal with this challenge. Recently, response surface techniques are used to model input and output relations of a given system to replace the conventional numerical analysis tool with a functional representation of the performance surface [33-35]. The intention is to minimize the computational time. Response surface techniques are applied to EM designs such as electromagnetic actuators [36]. Fast numerical EM methods are applied for electromagnetic modeling and simulation [37-39]. For example, patch antennas are designed with kriging and divided rectangles (DIRECT) method by E. S. Siah [40]. Lately, space mapping (SM) concept is introduced which exploits coarse models (usually computationally fast circuit-based models) to align with fine models (typically CPU intensive full-wave EM simulations) [41-48]. Other methods for speeding up the reanalysis are employed such as singular-value decomposition, which drastically reduces the order of the eigen-value problem. By inspection of the singular values, the accuracy level of the procedure may be controlled. The technique is applied to the analysis of open and closed waveguides with arbitrary cross section, lossy conductors, and anisotropic dielectric layers [49]. Recently, a framework is constructed where modeler and simulator interact through a distributed environment, (using established grid computing techniques) thus decreasing model generation and simulation turnaround time [50].

Different surrogate modeling methods such as Polynomials, Multiquadrics [51], Kriging and Artificial Neural Networks (ANNs) [52] are among approximation schemes or surrogate modeling techniques that exist in literature. The 'virtual' objective function they provide can be called by the optimization algorithm within a design optimization cycle. Many Response Surface Methods and combinations thereof are documented recently coupling especially the aforementioned approximation techniques with stochastic algorithms. Some methods are based on extrapolating local information [53] while others are solution technique dependent such as Chebyshev interpolations applied to enhance the efficiency of the moment matching technique [54]

Several factors exist in choosing the most appropriate surrogate model. These include the complexity and functional characteristics of the analysis model to be replaced and the effort in determining the surrogate model. In this thesis we compare the performance of different surrogate models in approximating the frequency response of electromagnetic devices to make that choice easier for similar design optimization studies. Mostly used surrogate models are polynomials, Radial Basis Functions (RBF), Kriging, Neural Networks and Support Vector Machines (SVM).

Polynomial models, [55-57] seem to be one of the natural choices for resonance based surrogate-modeling of electromagnetic devices since transfer functions of EM devices can in principle be represented by a rational function in the frequency domain. Polynomial models are fairly easy to implement, clear on parameter sensitivity, and cheap to work with but are usually less accurate than the Kriging model [40]. However, polynomial functions do not interpolate the sample points and are limited by the chosen function type. Similarly, RBF methods [58-59] are very popular for scattered data interpolation. They try to approximate available data a sample by a linear combination of translates of a single basis function. The main advantage, compared to polynomial models, is that they can handle huge amounts of data points. On the other hand, computations involving RBF quickly become infeasible as the dimension of the input space increases. Unlike rational functions they lack a theoretical connection with the physical problem at hand, so one would expect less favorable results when using RBF for surrogate modeling. Similarly, the RBF based surrogate models especially the multi-quadric RBF are easy to construct and can interpolate sample points at the same time. The advantage of the RBF is a provable non-singularity of the resulting linear problem, which makes RBFs especially useful in the model construction where multi-parametric models are involved. Regarding Kriging, more accurate models especially for nonlinear problems are usually obtained but these models are difficult to obtain and use, because global optimization is needed to identify the maximum likelihood estimators. Kriging is also flexible in either interpolating the sample points or filtering noisy data. Successful implementations exist in literature for a limited number of design variables [40]. Neural networks, on the other hand, are widely used in the field of statistics to automatically build models describing complex relations between input and output with a low computational cost. The basic principle of neural networks is to create an approximation of a complex function by combining simple elementary functions. In addition, it is known that Kriging and RBF are more sensitive to numerical noise than polynomial models. Finally, support vector machines (SVMs) are a set of related supervised learning methods used for classification and regression. They belong to a family of generalized linear classifiers. A special property of SVMs is that they simultaneously minimize the empirical classification error and maximize the geometric margin; hence they are also known as maximum margin classifiers.

1.5 Contribution and Overview of the Thesis

As the variety of examples in the literature shows, perfect combination of materials is unique and extremely difficult to determine without optimization. To address this issue, in this thesis we develop a surrogate model assisted design optimization framework integrating FEM based analysis tools with optimization techniques suitable for designing RF devices made of artificial magneto-dielectrics. Previous optimization studies on metamaterials indicate that properly designed dielectrics or a combination of different materials can lead to designs which have greater bandwidth and small size [10], [11]. Nevertheless, the focus has been on dielectric composites with two or more constituent ceramic mixtures relying on local optimization methods or global design search studies with restricted design capability. Here, our goal is to propose an efficient framework suitable to optimize the metamaterial profile fully, possibly with dielectric shades combined with magnetic materials to improve antenna performance such as miniaturization, bandwidth and efficiency within global design search studies. The need for design, preferably design optimization is pertinent to the competing physics of these metrics. Instead of the more traditional approaches of optimizing the shape or geometry of the antenna with numerical FEA based analysis tools, here we investigate the possibility to replace the FEA based model within material based designs and inverse topology optimization methods that could lead to non-intuitive magneto-dielectric substrates. When compared with more conventional optimization, where the topology of the device is assumed a priori and remains fixed, topology optimization offers much more degrees of freedom and allows the exploration of 3D artificial magneto-dielectric composites. Consequently, it is reasonable to expect that resulting designs have novel configurations with much higher performance. In Chapter 2, the resulting framework is applied to the design of a micro-strip patch antenna and optical plasmonic nano-antenna design. The proposed design framework effectively combines surrogate based models of FEA with optimization techniques and should allow for increased flexibility in geometry and material specifications across three dimensions for electromagnetic applications. Chapter 3 discusses surrogate models for EM design. To allow for considerable speed-ups of the versatile automated design process proposed here, automated and adaptive Design of Experiment (DOE) scheme is employed over the design domain and various surrogate models are compared within the design framework with respect to their performance. Multiple surrogate modeling techniques are investigated such as Artificial Neural Networks (ANN), Radial Basis Functions (RBF), Support Vector Machines (SVM), Kriging, and Rational Model. In Chapter 4, surrogate models are integrated into proposed design optimization framework. Results show that the hybridized surrogate model based design framework allows for large number of design variables and suggests the effective and global exploration of the large-scale design space. Micro-strip patch antenna is optimized for bandwidth using surrogate model assisted design optimization framework. Antenna design is a topic of great importance in EM community and involves the selection of several physical parameters to satisfy multiple stringent performance specifications such as optimal gain, pattern performance, bandwidth, VSWR, etc. To address this issue, multi-objectivity is successfully integrated into the proposed framework for possibly bandwidth and gain improvements of a patch antenna.

Future work comprises the extension of the framework capabilities to the design of the microstructure of metamaterials utilizing inverse topology optimization. The possibility to explore all possible design degrees of freedom for the material itself is expected to open up entirely new possibilities in microwave and optical applications.

In short, the contributions of the thesis can be summarized as follows:

- An efficient multi-objective surrogate model assisted design optimization framework for RF and optical applications is developed.
- Proposed framework is applied to several designs including multi-layer microstrip patch antennas and optical plasmonic nano-antennas.
- Several surrogate model techniques are compared for EM design.
- As a result of developed framework, 80% CPU time saving is succeeded for large scale design optimization problems.

2 THEORETICAL BACKGROUND

2.1 Design Optimization

Generally design problems whether carried out intuitively or via optimization can be classified into size, shape, and topology optimization, where the design variables are proportions, boundaries, and topology of a component, respectively. Optimization is the process of maximizing or minimizing a desired objective function while satisfying a set of constraints. A design optimization cycle typically consists of a synthesis module and an analysis module. The synthesis module contains a specific optimization algorithm and the analysis module computes the objective function and its derivatives, if a sensitivity analysis is required by the chosen optimizer. Most optimization algorithms are iterative methods and have their own way of searching towards the optimum solution. Specifically for antenna design optimization problems, the desired performance characteristics are described and formulated in terms of an objective function, such as bandwidth, beam angle, frequency response, efficiency or similar. The analysis module usually consists of a finite element analysis code, since the antenna structure and boundaries are complex for deriving a closed-form solution satisfying Maxwell's equations.

Mathematically, an optimization problem can be defined as follows:

$$\begin{aligned} &\text{Minimize: } f\,(\mathbf{x}, \mathbf{p}) \\ &\text{Subject to: } \mathbf{g}(\mathbf{x}, \mathbf{p}) \leq \mathbf{0} \\ &\mathbf{h}\,(\mathbf{x}, \mathbf{p}) = \mathbf{0} \end{aligned} \qquad (2.1)$$

Where $\mathrm{x} \in x \subseteq R^n, f : R^n \rightarrow R, h : R^n$ and $g : R^n \rightarrow R^s$. Here (2.1), **x** is the design variable vector in the design space $\boldsymbol{x}$, the vector **p** contains certain parameters with values fixed during optimization. f(**x, p**) is the objective function, the **g** (**x, p**) vector is a set of inequality constraints and **h(x, p)** denotes the equality constraints. The set of x that satisfy all constraints is called the feasible region.

In the most general form, the above formulation is a constrained nonlinear programming (NLP) problem. Optimization problems can be classified in several ways such as constrained or unconstrained problems, integer or real-valued programming problems, and component or system design optimization problems, etc. Most well known classification is to differentiate them whether or not they rely in the evaluation of gradients as gradient based/local or global/heuristic techniques and are discussed next.

2.2 Gradient Based Optimization Techniques

It is fair to say that these techniques usually require less number of iterations when compared with global techniques and hence are faster. These algorithms make use of first and generally the second derivative of the objective and constraint functions and use this information to locate the optimum. One disadvantage is their dependence on the starting point of the search. At that point the user is responsible of making a clever guess and defining a good starting point to find the optimum point. Their biggest disadvantage is getting stuck at a local optimum unless certain conditions such as convexity are not satisfied. At each n^{th} step of a gradient based optimization algorithm a new iterate x_{k+1} will be suggested based on the previous iterate x_k , a move step α_k and a search direction s_k as follows:

$$X_{k+1} = X_k + \alpha_k s_k \tag{2.2}$$

The iteration goes on until a specific convergence criterion is met such as the difference of successive iterates dropping below a small number ε. Another common termination criteria is the Karush-Kuhn-Tucker norm such as:

$$\|\nabla f_k + \lambda_k^T \nabla h_k + \mu_k^T \nabla g_k\| \leq \varepsilon \tag{2.3}$$

Classical gradient based methods for unconstrained non-linear programming problems include: Cauchy, conjugate gradient and quasi-Newton methods. Among the most popular one Sequential Quadratic Programming will stand out as a successful technique to effectively solve problems with nonlinear constraints and is employed in the design framework as the local optimization technique.

2.2.1 Sequential Quadratic Programming (SQP)

SQP is based on the idea of reducing the complexity of the problem by sequentially solving less complex quadratic sub-problems with gradient methods. As the complexity of the original problem is reduced this method is expected to be faster to solve the original non-linear problem. For a given optimization problem as:

$$\begin{gathered}\text{Minimize } \mathbf{f}\,(\mathbf{x}) \\ \text{Subject to } \mathbf{h}(\mathbf{x}) = \mathbf{0} \\ \mathbf{g}(\mathbf{x}, \mathbf{p}) \leq \mathbf{0}\end{gathered} \qquad (2.4)$$

Where f($\mathbf{x}$) is the nonlineqar objective function, g($\mathbf{x}$) is the nonlinear constraints, and h(x) is the vector of linear equality constraints.

Again the iteration stops when an optimum is reached in the standard gradient based optimization setting and follows below steps:

1) Initialize the system.
2) Solve the problem stated in (2.4).
3) Minimize a merit function along s_k by performing a line search to determine the step length α_k
4) Set $x_{k+1} = x_k + \alpha_k s_k$
5) Check for termination, go to step 2 if not finished.

In the proposed framework the SQP algorithm in MATLAB has been used.

2.3 Heuristic Methods

Gradient based techniques as described above for SQP are highly likely to converge to a local optimum depending on the characteristics of the optimization problem and the choice of the initial design point. In contrary, heuristic methods do not rely on local information such as the gradient and hence have the capability to search for global optima. Basically heuristic methods scan on a larger design space with increased boundary, and in return rely mostly on many more computations, hence suffer usually from slow convergence and impractical design time spans. This computational burden is even more pronounced for design problems with high number of design variables such as topology design efforts of frequency based electromagnetic problems. Most common design optimization studies within the electromagnetic community have been restricted to the use of heuristic methods such as the genetic algorithm to parametric design studies. Basic principles of GA's will be introduced next. Applications of GA's exist in a wide range of application portfolio ranging from the high speed integrated circuit to the simulations of the electromagnetic materials. There is no guarantee that it always converges but practical applications suggest that it is usually quite successful in dealing with complex design problems.

2.3.1 Genetic Algorithms

Genetic Algorithm (GA) is a robust intelligent optimization algorithm that gives the global optima without the need for the derivative properties of the function with the usage of a system that mimics the behavior of the nature population's genetics and evolution.

In a genetic algorithm every species represents a variable in the problem. The algorithm seeks for the fittest of the individuals by combining the individuals from each species with each other randomly. The algorithm continues to choose the individuals to breed until it finds the fittest in the population. Once it locates the fittest in one population it continues to breed the populations until it finds the fittest in the subsequent population. This process of mixing individuals is similar to the process of crossover in nature.

In a standard GA setting, the user chooses certain parameters such as the size of the initial population, mutation ratio, and crossover ratio. The reason for the need of the mutation is to introduce diversity and prevent the design candidates to be too much ‘alike’, i.e., distributed homogenously within the population which reduces the quality of the search and hence the results of the algorithm. So, at some generations, the individuals are changed/renewed to prevent too similar design candidates. The fitness criterion is also defined by the user, which itself is a challenging task for any optimization model.

A new generation is started each time until a termination condition has been reached. Termination criteria include:

- A solution is found that satisfies minimum criteria,
- Fixed number of generations reached;
- Allocated budget (computation time) is reached;
- The highest ranking solution's fitness is reaching or has reached a plateau such that successive iterations no longer produce better results;
- Manual inspection;
- Combinations of the above.

In general, although GA is very capable of providing good solutions to difficult problems, they offer no guarantee of global optimality in finite time. They are very sensitive to tuning parameters and they don`t eliminate risk of premature convergence.

2.4 Analysis Tools

Complex structures such as patch antennas require to be solved via numerical tools such as with finite element analysis. The finite element analysis is a numerical technique for finding approximate solutions of partial differential and integral equations. The solution approach is based either on eliminating the differential equation completely (steady state problems) or rendering the PDE into an approximating system of ordinary differential equations (ODE), which are then solved using numerical techniques such as Euler's method and Runge-Kutta etc.

In our studies we used two FEM based analysis tools: FSDA (Fast Spectral Domain Algorithm) and HFSS (High Frequency Structure Simulator).

2.4.1 Fast Spectral Domain Algorithm (FSDA)

FSDA is used to analyze electromagnetic scattering and radiation characteristics of infinite periodic planar antenna arrays and frequency selective surface (FSS: metallic/resistive patch or slot elements), as illustrated in Fig. 2.1, or frequency selective volume (FSV: metallic or dielectric block inclusions) configurations, with an arbitrary number of FSS/FSV layers, or combination of both antenna arrays and FSS/FSV configurations. The code is capable of dealing with commensurate as well as non-commensurate structures.

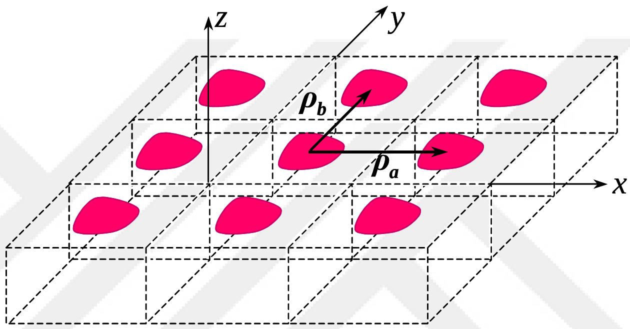

Fig. 2-1 Metallic/resistive patch or slot elements

The hybrid finite element/boundary integral (FE/BI) method is used for field calculation. The finite element formulation is employed within the volumetric part and the boundary integral is used for terminating the mesh. The code works with prismatic elements (right-angled) in the FE-sector and triangular elements in the BI-surface. First, the code generates triangular surface meshes with all geometrical adaptability for the individual layers while the volumetric FE mesh is grown along the depth of the volume. The code has the option to deal with metal-backed periodic configurations and with periodic configurations which are open at the top as well as at the bottom surface of the FE-mesh. In the first case, the BI is applied only on the top surface whereas in the latter, the BI-method is used to terminate both surfaces.

To model the infinite array problem, the periodicity condition for the fields in the infinite periodic array is employed using only one unit cell of the array. That is, within the FE-model of this unit cell, the periodic boundary condition (PBC) is enforced on the vertical walls of the mesh and on the boundary edges of the BI-surfaces where also an appropriate periodic Green's function (PGF) must be used. For modeling non-commensurate structures, the individual layer periodicities are decoupled. Of course, this is only an approximate model but its accuracy can arbitrarily be improved by grouping several cells in the individual layers [60].

In this study, the FE-BI based code is integrated within the proposed design framework using a Matlab interface and applied to 3 layer micro-strip patch antenna for bandwidth optimization.

2.4.2 High Frequency Structure Simulator (HFSS)

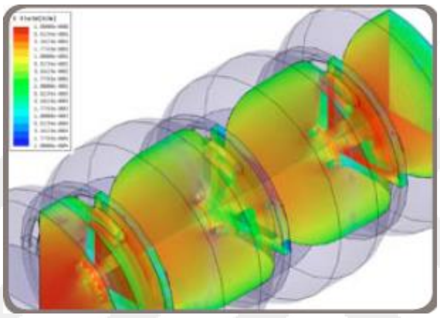

Fig. 2-2 A graphic from HFSS program.

HFSS is the industry-standard software to analyze electromagnetic structures. It utilizes 3D full-wave Finite Element Method (FEM) to compute the electrical behavior of high-frequency and high-speed components. With HFSS, network parameters (S, Y, Z) can be extracted, 3D electromagnetic fields can be visualized, broadband SPICE models can be generated, and optimize design performance. The software is widely used for the design of on-chip embedded passives, PCB interconnects, antennas, RF/microwave components, and high frequency IC packages. HFSS characterizes the electrical performance of components and evaluates signal quality, including transmission path losses, reflection loss due to impedance mismatches, parasitic coupling, and radiation.

The graphic interface of HFSS allows designing various kinds of geometric shapes, 1D, 2D, or 3D from its drawing tools. It also gives the opportunity to create different kinds of analysis on the same model without any interaction with each other. [61].

HFSS software is an easy to use one, especially the combined usage of it with the Matlab toolbox gives the users the chance to work on a variety of fields. As it uses

Microsoft Graphical User Interface for windows the designer can see his exact design in three dimensions. It also gives the freedom to calculate performance metrics for a wide range of frequencies which makes it suitable especially for antenna designs and high speed integrated circuits. Moreover, adaptive meshing is possible for complex geometries which make it suitable for iterative based design studies. These features and the convenient script recording feature are among reasons HFSS has been chosen as the primary analysis model for the proposed design optimization framework. It is used for the design of plasmonic nano-antennas, micro-strip patch antennas, and surrogate model comparisons in this thesis.

The main idea of HFSS scripting is based on the ability of recording design steps into a script file and that script file can be converted into a Matlab file. That gives the user the opportunity to work on Matlab, call HFSS from Matlab and do the design steps automatically. In the script the user can assign variable names to some critical settings like the frequency sweep range, permeability, permeability of a user designed material and that makes it quite easy to call the necessary files and each time evaluate the antenna for a different design setting. Also the results can be exported to an external environment like a text file and they can be read by Matlab to be fed into optimization module which is discussed next.

3 FEA BASED AUTOMATED DESIGN OF ANTENNAS

3.1 FSDA based Design Optimization Framework

In this section the basic structure of the proposed design framework is summarized. The modular structure of a standard design framework for material based design efforts is shown in Fig. 3.1. The analysis tool within the framework is the commercial Ansoft HFSS package. Since design optimization requires successively changing design variables at each iteration, an API is needed to integrate HFSS with the framework. After an intensive search, an appropriate HFSS-Matlab API library, we found a suitable library. To demonstrate the framework as the first example a patch antenna is programmed thru HFSS tutorial and results are validated with HFSS GUI. Afterwards, the optimization module such as GA/SQP and the analysis module HFSS are linked to each other. This forms the design optimization cycle. Initial efforts to apply the gradient-based optimization to a design example were not successful primarily due to slowness of HFSS, hence sensitivities could not be evaluated with enough accuracy in a feasible time. This motivated the use of HFSS based reduced models and details of the model reduction strategies and its use in the design framework are discussed in the third and forth chapters.

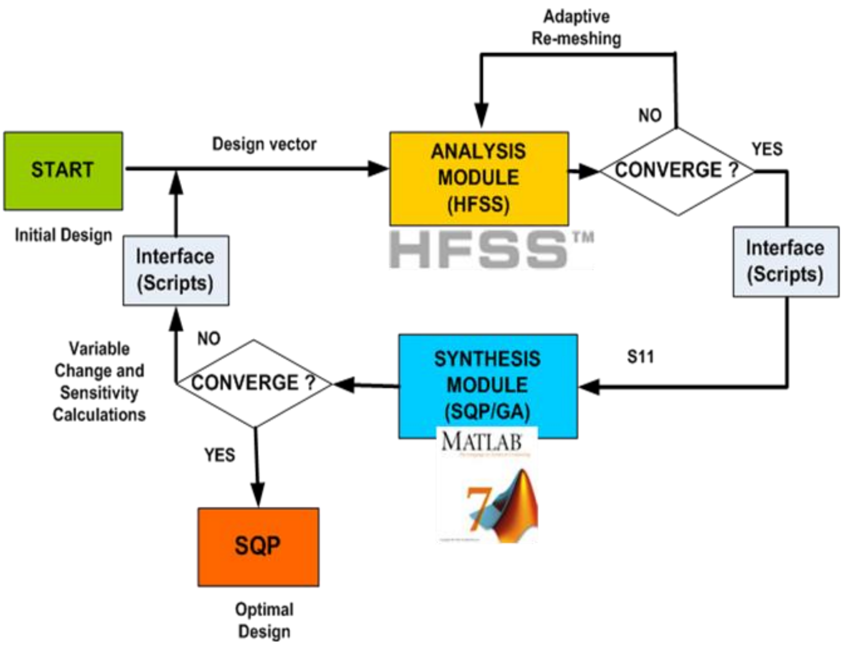

Fig. 3-1 Matlab based design optimization framework

3.2 Design Example 1

3.2.1 Magneto-Dielectric Optimization of a Multilayer Patch Antenna

In this section we demonstrate a parametric design optimization study for magneto-dielectrics substrates using the proposed design optimization framework. The goal is to determine optimal values of the permittivity and permeability of each magneto-dielectric layer supporting a probe fed patch antenna subject to high bandwidth and size constraints. Main motivation is to use resulting optimal values as objective metrics to be attained subsequently via inverse homogenization as discussed earlier. Among future goals is to determine the microstructure of each layer subject to effective material properties resulting from the pre-design phase presented here. Chosen microstrip patch antenna consists of 3 magneto-dielectric layers. Geometrical details are shown in Fig. 3.2. The allowable permittivity and permeability range is [1-25]. The objective function is chosen as $f(x) = \min[\max(|s_{11}|_i)]$ where $i = 1,\ldots,N_{freq}$, $\mathbf{x}$ is the design vector and s_{11} is the return loss. Design specifications are shown in master table (Table 3.1).

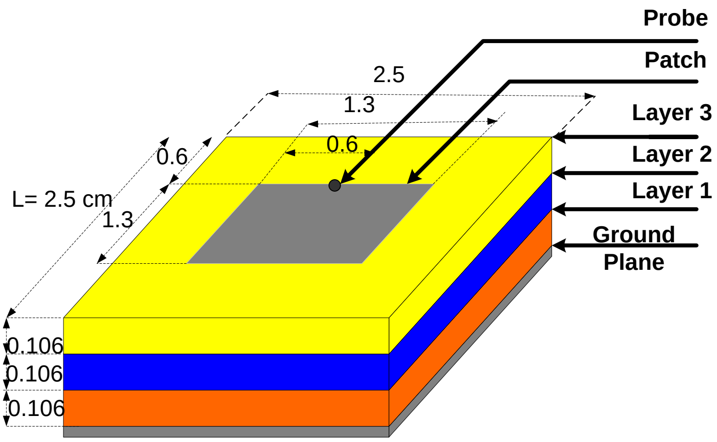

Fig. 3-2 Multi-layer patch antenna geometry.

The antenna is analyzed via full wave FE-BI tools to compute return loss (S_{11}) values. The optimization scheme chosen here is Sequential Quadratic Programming. Target is to attain bandwidth performance enhancements by changing the material properties of the dielectric layers. Their optimum composition will be found subsequently via inverse topology optimization. From this point of view, the magneto-dielectric layers here can be treated as effective material properties.

Master Table/ Description	Symbol	Description	LB	UB	Initial value	Unit
Design varible-1	x(1)	Eps_L1	0	100	3	F/m
Design varible-2	x(2)	Mu _L1	0	100	3	µN/A2
Design varible-3	x(3)	Eps _L2	0	100	3	F/m
Design varible-4	x(4)	Mu _L2	0	100	3	µN/A^2
Design varible-5	x(5)	Eps_L3	0	100	3	F/m
Design varible-6	x(6)	Mu _L3	0	100	3	µN/A^2
Parameter 1	W*L	Antenna size	n.a	n.a	(2.5,2.5)	cm
Parameter 2	PS	Patch size	n.a	n.a	(1.3,1.3)	cm
Parameter 3	PP	Patch position	n.a	n.a	(0.6,0.6)	cm
Parameter 4	NL	Number of layers	n.a	n.a	3	cm
Parameter 5	PP	Probe position	n.a	n.a	(1.9,1.3)	cm
Parameter 6	PC	Probe current	n.a	n.a	1	Amper
Objective	J	S11	n.a	n.a	0	db

Table 3.1: Master table of antenna design.

The optimal values of their properties resulting in the ‘best’ bandwidth performance subject to the chosen optimization model are evaluated using a SQP algorithm and the full wave analysis tool (Fig. 3.3). Initial design refers to a homogeneous dielectric substrate with ε = 3 and µ = 3. Operating frequency range is chosen as 0.5 GHz - 3 GHz sampled with 0.1 GHz intervals. Optimization results are shown in Fig. 3.4 and 3.5. Convergence was reached in about 35 iterations. As apparent, the initial design structure doesn't have a resonance in the desired working frequency range, whereas the optimal design delivers a -5dB bandwidth. With the attained improvement with only 6 design variables and pre-chosen antenna geometry, the results clearly demonstrate the positive effect of artificial magneto-dielectric substrates on the bandwidth of the micro-strip patch antenna. A design search considering the conducting patch as well, i.e. the integration of the conductivity of each layer should allow for much wider bandwidth. It is also noted that the chosen objective function is not favoring matched performance but rather just bandwidth. A more suitable objective function could be employed to aim for well matched behavior. The next step could be to feed the resulting ε and μ values (ε_1=8, μ_1=2.45, ε_2 =5.8, μ_2 =15.9, ε_3 12.5, μ_3 =2.6) into the inverse topology optimization scheme to explore the layer microstructure that can deliver desired effective material properties.

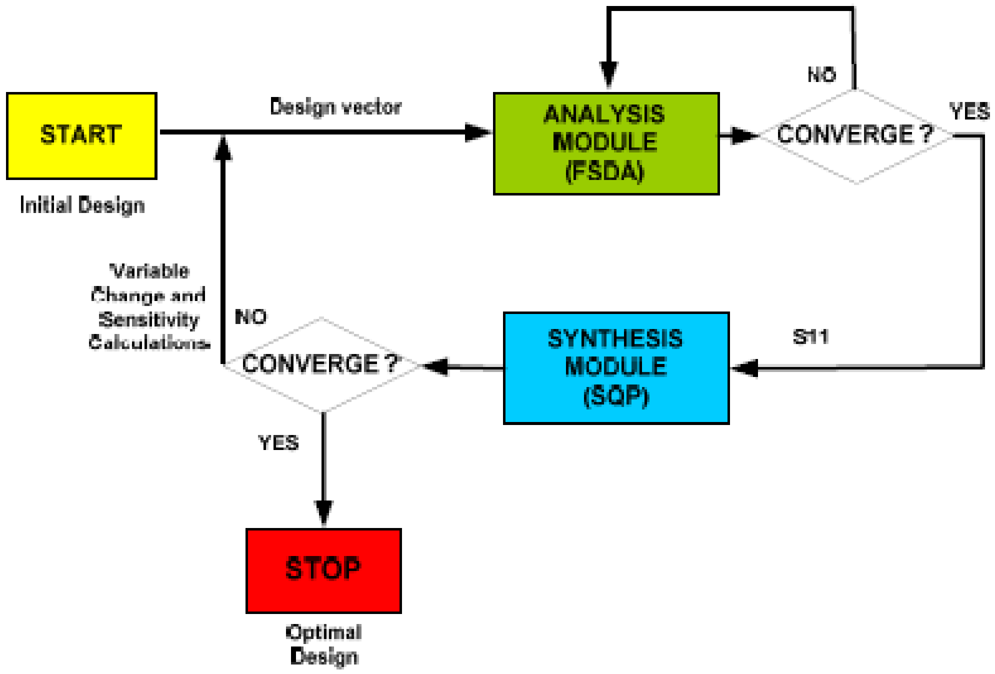

Fig. 3-3 Design optimization framework

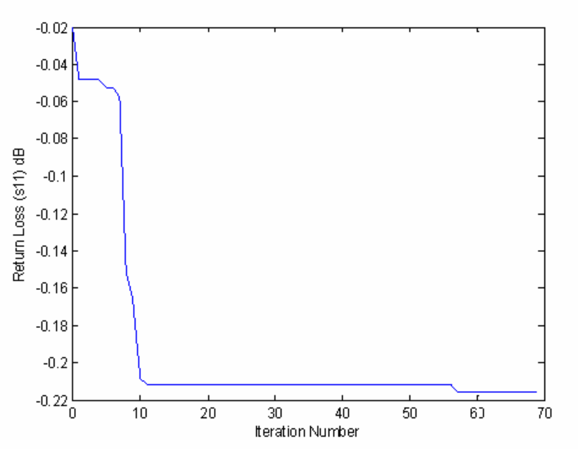

Fig. 3-4 Optimization history

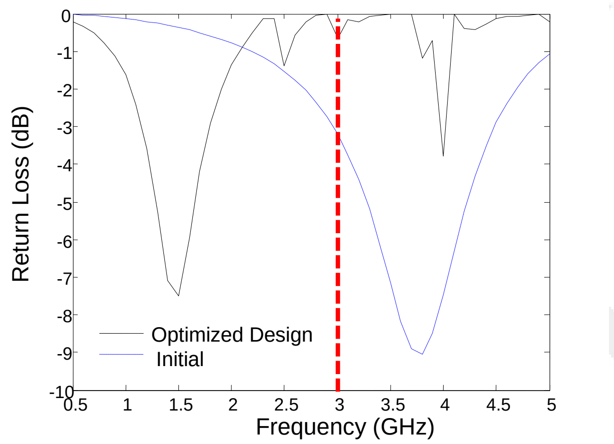

Fig. 3-5 Initial vs. optimized bandwidth performance

The resulting bandwidth although much higher than the initial design could correspond to a local optimum value hence allow for further bandwidth improvements. To arrive at global optimal design solutions possibly via a two-step large scale design optimization approach subject to performance metrics calculated at sampled frequency points, heuristic search routines need to be employed. The proposed framework is flexible enough to be solved via evolutionary optimization techniques to address this issue, if appropriate speed-up techniques are adopted. These techniques are discussed in the next chapter.

3.3 Design Example:

3.3.1 Optimization of a Nano-plasmonic Antenna

Nano-optical applications, such as scanning near-field optical microscopy [62] and data storage [63], require intense optical spots beyond the diffraction limit. Nano-antennas [64-65] can obtain very small optical spots, but their ability to obtain optical spots beyond the diffraction limit is not sufficient for practical applications. In addition to a very small optical spot, a nano-antenna should provide high transmission efficiency for practical applications. The transmission efficiency of a nano-antenna determines the data transfer rate of storage devices and scan times of near-field optical microscopes. Therefore, the efficiency of nano-antennas should be optimized for potential utilization in practical applications. Optimization of nano-antennas is crucial for understanding their potential and limitations for emerging plasmonic applications. A brute-force optimization study of these structures is not practical due to large number of parameters. There is a need for a systematic optimization of these structures.

In this study, the proposed design framework is used to optimize nano-antennas.

3.3.1.1 Dipole and bow-tie plasmonic nano-antennas

An antenna is composed of metallic parts. For example, the dipole antenna shown in Fig. 3.6(a) is composed of two metallic rods separated by a distance, *G*. Similarly, a bow-tie antenna shown in Fig. 3.6(b) is composed of two triangular metallic pieces, which are also separated by a distance, *G*.

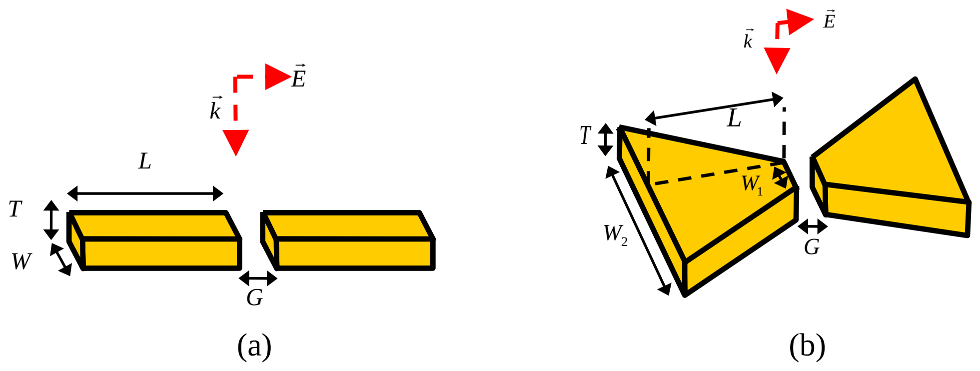

Fig. 3-6 A schematic illustration of a (a) dipole and (b) bow-tie antenna, and their dimensions. The antennas are illuminated with incident electromagnetic radiation shown with $\vec{E}$.

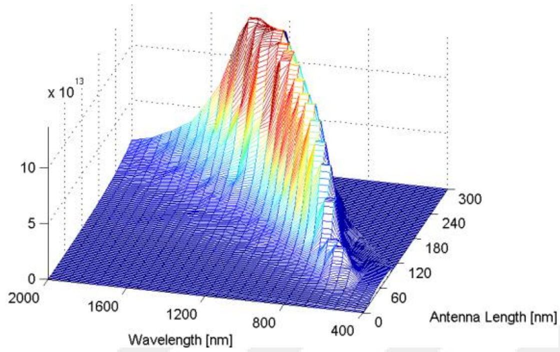

Fig. 3-7 The intensity as a function of wavelength and antenna length for: *T*= 50, *W*= 50, and *G*= 20 nm.

For the purpose of exploration of the design domain, some simulations are done. The incident wavelength is varied from 400nm to 2000 nm by intervals of 50 nm, At each wavelength, antenna length is changed. The intensity at the center of the gap, $|E(x=0, y=0, z=0)|^2$, is calculated for each wavelength and antenna length. By recording the intensity over the rectangular grid shown in Fig. 3.7, the surface graphs are formed. A constant power value of 1 mW is chosen. The power calculations are based on a focused beam model. More information can be found in Handbook of optical constants of solids by E.D. Palik, 1998

3.4 HFSS based Design Optimization Framework

The surface plasmon resonances of nano-antennas depend on parameters related to the shape and composition of the nano-antenna. Complete understanding of surface plasmon resonances of nano-optical systems requires a complete and detailed understanding of possibly many more design parameters, geometries, and material properties. The large number of parameters involved in studying functional plasmonic devices with a brute force numerical parameter simulation is not feasible. To design novel nano-optical transducers a modeling based automated design optimization framework is necessary.

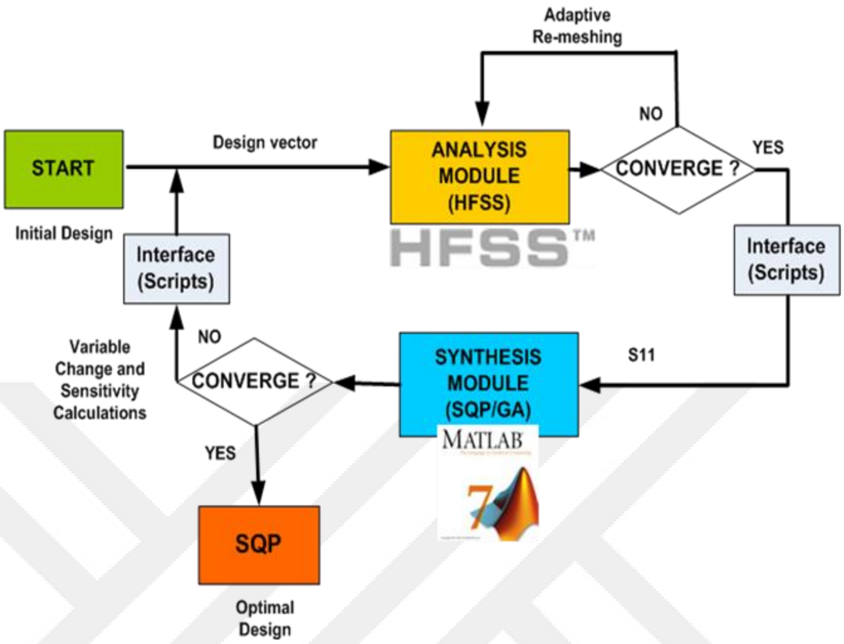

Fig. 3.8 Design optimization framework for nano-antenna design

The design framework is formed by integrating a commercial electromagnetic analysis tool Ansoft HFSS with MATLAB’s optimization toolbox. Specifically, two different optimization tools are integrated on a MATLAB based scripting interface to iteratively search for optimum geometric parameters of a dipole and bowtie antenna: sequential quadratic programming (SQP) and genetic algorithm (GA). The optimization model consists of maximizing the field intensity $|E(x=0, y=0, z=0)|^2$ subject to bound constraints of [20, 450] and [400, 2000] for geometric length and wavelength, respectively. Convergence is achieved in about less than 20 iterations and 10 generations for the SQP and GA framework, respectively. Optimization parameters in the GA setting include 10 individuals, Gaussian Mutation and Roulette Wheel Selection. Optimal lengths for dipole antennas are obtained via SQP, plotted with respect to wavelength, and compared to results obtained via the brute-force simulation in Fig. 3.9. There is an overall agreement except for optimal lengths at wavelengths close to bound constraints. The discrepancies are attributed to two main reasons: Inaccurate brute-force predictions of maximum field intensity of finite sampled frequency points and as expected with gradient based optimization tools, results show that SQP's performance in locating the optimum solution depends on the chosen initial design with especially when the intensity is a multi-modal function. The GA based optimization framework seems to overcome this issue in the expense of computational time. Optimal results for the bow-tie antenna length converged to 140 nm at 900 nm, and to a dipole length of 286 nm at 1764 nm for a two variable optimization study via the GA framework while the SQP was unable to converge for the latter. Initial results seem to be promising in providing the capability of exploring nano-structures with several design parameters. The electric field performance is likely to result in more complicated response functions. Future work includes expanding the framework to hybridize both optimization tools in combining the advantages of global and local optimization tools and to expand the framework to multi-objective design optimization problems.

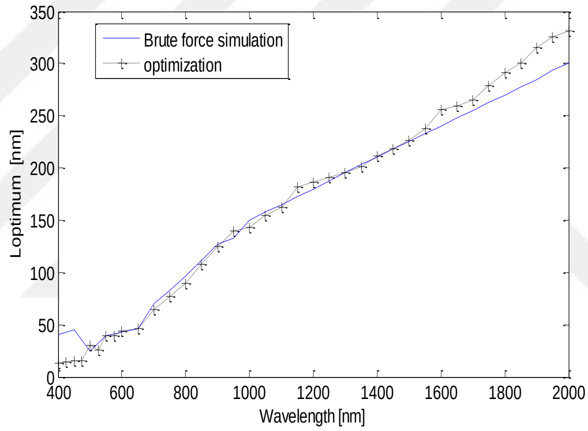

Fig. 3.9 Comparison of the optimization result for a dipole antenna using the SQP method and brute-force simulations.

Design optimization framework is also applied to the case where the power is taken to be constant, and wavelength and rod length are allowed to change. GAs has been chosen as the optimization algorithm. Length is allowed to vary in a range of 10-300 nm and frequency is allowed to vary in a range of 150-750 Thz. Results are satisfactory and shown in Fig 3.10.

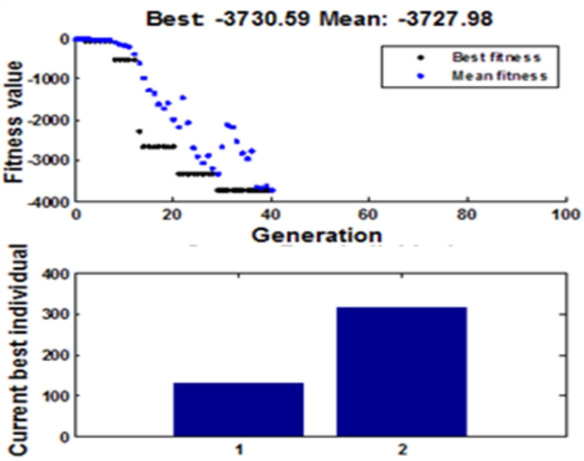

Fig.. 3.10 GA result of constant power nano-antenna optimization

Bowtie Antenna is optimized with the proposed framework using GA as optimizer. GA converged to Lopt: 190 [nm] in 550 function calls finding global optimum (Fig 3.11), SQP converged to Lopt: 250 [nm] in ~20 function calls (converged prematurely).

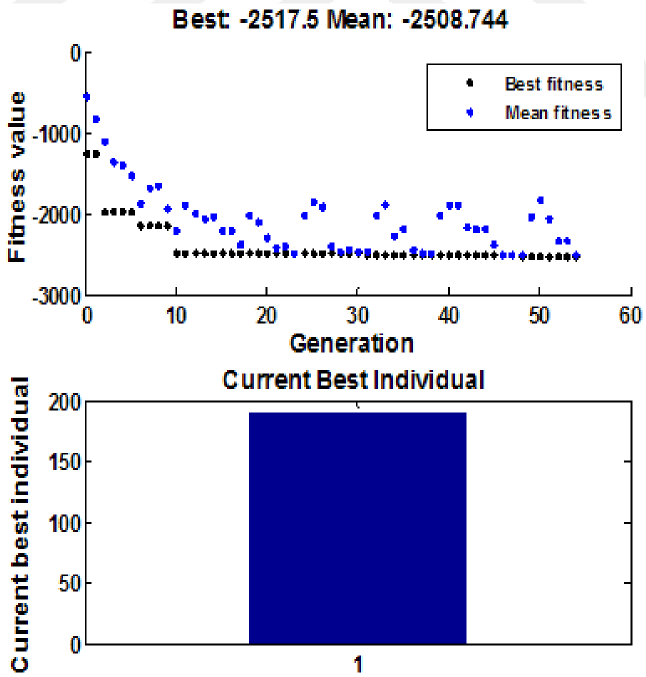

Fig. 3.11 Bowtie nano-antenna optimization with GAs

4 SURROGATE MODELING BASED DESIGN OPTIMIZATION

4.1 Introduction

Large scale design optimization problem often involve a broad design space and computationally expensive simulations. Many detailed FEM based analysis tools are available for use in the latter stages of EM design, but they are extremely expensive for exploring broad design regions. One solution has been to simplify the computational cost of analysis models by reducing the finite elements model, or increasing the step length within frequency sweeps to obtain approximate simulation results. Thereby, accuracy is sacrificed and computational time is reduced. However, exploring large design domains and performing design optimization based on repetitive approximate simulations could be still costly. To overcome this computational challenge, surrogate models are created to provide rapid approximations of more expensive finite element based models. Previous studies as discussed in Chapter 2, showed that large scale design optimization problems such as multilayer patch antennas and nano-antenna based design optimization, require large amount of computational resources.

Creating surrogate models for EM design requires following specific set of actions. First, finite element method (FEM) based computer experiments are performed, chosen in specific patterns called experimental designs [66,67] in which the design variables cover a chosen range of values. Using chosen analysis module, design's performance is simulated at chosen sample points. The responses and input values are evaluated statistically to create functional relationships between input variables and performance functions of the design. These functional relationships are called surrogate/meta- models. These surrogate models can be used to explore the design domain, linked to an optimization framework and used to replace the analysis tool and guide the optimization process.

There is a wide variety of methods available for surrogate modeling [68]. Among them are artificial neural networks ANN, radial basis functions (RBF), kriging, Support vector machines (SVM) and polynomials. Success of surrogate modeling is determined by several factors such as the choice of the surrogate modeling method, used error measure, the experimental design used to select data points, the size of the design space or range of explored values of design variables, the accuracy of the simulation at each data point and the numbers of data points available to compute the surrogate model. In this work, we will explore ANN , Kriging, RBF and SVM methods for modeling Electromagnetic behavior based on the error value of the built metamodel also qualitatively since over-fitting is a know issue with metamodels.

4.1.1 Sampling Design Space via Design of Experiments (DOE)

For the purpose of developing an accurate approximation of the design domain, the sampling from domain must be based on an intelligent scheme. The accuracy of the approximation model and the duration for obtaining it is determined by the chosen sampling scheme so it would be wise to use an effective one.

Design of Experiment (DoE) is a structured, organized method that is used to determine the relationship between the input factors affecting a system and the output of that system. This method was first developed in the 1920s and 1930, by Sir Ronald A. Fisher who is a renowned mathematician and geneticist.

Design of Experiment involves designing a set of experiments, in which all relevant design variables are varied systematically. When the results of these experiments are analyzed, they help to explore the design domain, the variables that most influence the results, and those that do not, as well as details such as the existence of interactions and synergies between factors. In our study, we will use DOE for surrogate modeling. There are various DOE techniques such as Central Composite Design (CCD), Latin Hypercube Design, Orthogonal Arrays, etc. Here, latin hypercube design is used: Latin Hypercube Design method is one of the cleverest way of searching in an n dimensional design space An experimental design consisting of n trials, and for which each factor has n distinct levels.

4.1.2 Generation of Surrogate Models

Our goal is to compare various surrogate modeling methods for their suitability within a versatile design optimization framework developed for electromagnetic applications. The ultimate design optimization framework is based on integrating hybrid design optimization techniques with various surrogate modeling tools towards the goal of designing volumetric material and conductor variations of complex electromagnetic devices. The framework will be utilized to identify the novel device structure from scratch, both its material and conductor variation in three dimensions, in an automated and efficient manner subject to some performance and size constraints. For the synthesis module, gradient-based optimizers such as SQP and global optimizers such as Genetic Algorithms are both utilized. As the analysis module, full wave electromagnetic wave solvers, both a commercial EM simulator, Ansoft HFSS, and an in-house hybrid FE-BI based analysis tool are utilized. The design framework is primarily based on interfacing the analysis tools with various surrogate based models and linking it to the optimization tools.

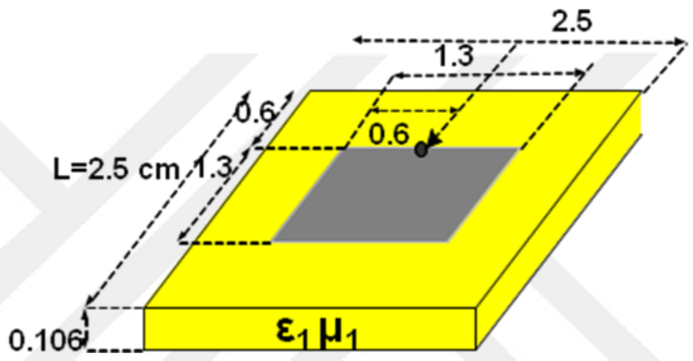

Fig. 4-1 Antenna Model of the Surrogate Model (Dimensions are in cm)

To investigate the performance of aforementioned surrogate models on the same design problem, surrogate models are applied to approximate the return loss response of a simple patch antenna with a magneto-dielectric substrate as shown in Fig. 4.1. The antenna is analyzed via Ansoft HFSS v11 to compute its frequency based return loss (s_{11}) response. The permittivity and frequency are chosen as design variables. Permittivity of the substrate is allowed to vary 1-16. Frequency band of operation is specified to be between 1-2.5 GHz. The permeability is chosen to be a fixed parameter with a value of $\mu = 2$. The reason of the choice of permittivity and frequency as design variables is to evaluate the fitted surface as qualitatively. Because it is well known that for one layer patch antenna, resonance frequency follows a special trend as permittivity changes. The geometry and probe position is hold fixed as parameters, not to effect the resonance frequency which is our guide towards evaluating the models accuracy qualitatively.

To allow for considerable speed-ups, an adaptive DOE scheme is integrated in an automated fashion to the surrogate modeling tools. The performances of five different models are compared within the same framework: Kriging, Polynomial, RBF (Radial Basis Functions), Artificial Neural Networks (ANN), and Support Vector Machines (SVM). Each surrogate model is constructed based on the outputs of the EM simulator for a limited number of intelligently chosen data points based on the DOE scheme. More specifically, surrogate models are created by integrating a commercial high frequency analysis tool, Ansoft HFSS with a MATLAB programming environment to automate the experiments which a DOE scheme requires. HFSS simulates the exact electromagnetic response of the device and the Latin Hypercube Method is used as the DOE scheme. It systematically investigates the system where a series of structured tests are designed in which planned changes are made to the input variables of the system. For the purpose of generating surrogate models, Surrogate Modeling Toolbox (SUMO) [72] is integrated with our automated DOE platform. In addition to the DOE scheme, adaptive sampling which is based on the combination of the accuracy of the model measured by root relative square error and density of the samples in the design domain is used with the goal of producing models with improved quality provided by SUMO.As a model validation metric, validation set (80% of sampling for training, 20% of sampling for validation) is used. Quality is measured in terms of error function which is defined as root relative square error (RRSE) calculated by

$$E = \sqrt{\frac{MDE}{Variance}} \tag{4.1}$$

Where MSE is Mean Square Error. MSE measures the average of the square of the error. Variance is one measure of statistical dispersion, averaging the squared distance of its possible values from the expected value. Error measure is set to 0.1. The less this value is, the better the model. However due to fast convergence it is set to be 0.1. The default value in SUMO is 0.05.

4.2 Surrogate Modeling Techniques

In this chapter we investigate five specific surrogate modeling techniques for their performance in speeding up the materials based antenna design problem exhibiting resonance behavior.

Each surrogate model has its own advantage and disadvantages. A quick comparison of each model can be found at Fig. 4.2. Artificial Neural Networks (ANN) is known to have the capability to model any nonlinear behavior. It requires low storage space. However ANN needs a lot of training examples. There are also over-fitting challenges related to the model. Support Vector Machines (SVM) is based on computational learning. Many training samples are required to obtain the model. SVM deals with multi-dimensional problems easily. Radial Basis Functions (RBF) is scale independent. There are many tuning variables and models success depends on the initial model. Polynomial fitting is simple and practical. It uses least squares. There are some boundary condition challenges related to it. Kriging is a rough approximation. Its theory depends on hyper dimensional least squares. It is independent of the RSM type. There are some strong assumptions related to it.

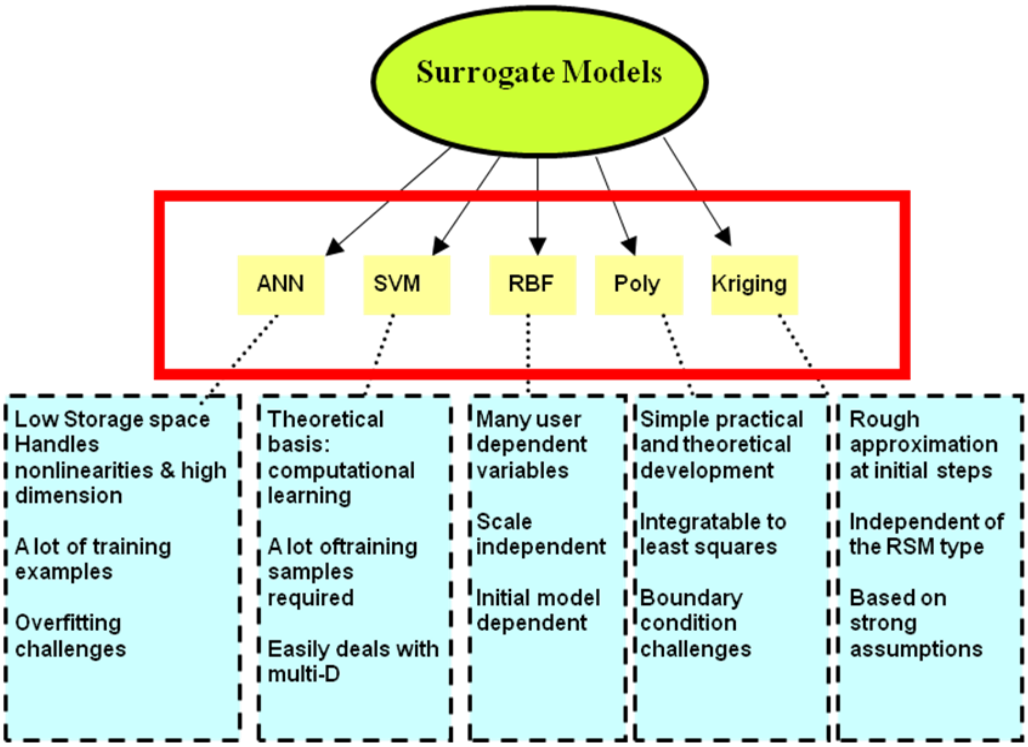

Fig. 4-2 Features of used Surrogate Modeling Techniques

In this chapter theories behind each surrogate model is expressed and the application results are given.

4.2.1 Artificial Neural Networks (ANNs)

Artificial neural networks (ANNs), are information processing systems inspired by the ability of the human brain to learn from observations and to generalize by abstraction [80]. ANNs can be trained to learn any arbitrary nonlinear input–output relationships from corresponding data. ANNs are used in applications such as pattern recognition, speech processing, and control systems. Recently, ANNs have been applied to obtain surrogate modeling approximations for design process requiring computationally costly simulations. Neural networks are first trained to model the response of the EM design. Costly simulations can then be replaced with these trained networks which will provide fast answers. Neural networks are efficient alternatives to conventional methods such as numerical modeling methods, which could be computationally expensive, or analytical methods, which are difficult or impossible to obtain for complex devices, or empirical models, whose range and accuracy could be limited.

A typical neural network structure has two basic components: processing elements (neurons) and interconnections (links/synapses) between them. Every link has a corresponding weight parameter (Fig 4.3). Each neuron receives stimulus from the neurons it is connected to, processes the input and returns an output as a response.

MLP is the most popular neural-network structure. In the MLP neural network, neurons are grouped into layers. The first and the last layers are called input and output layers, respectively, and the remaining layers are called hidden layers. Suppose the total number of layers is L. The first layer is the input layer, the lth layer is the output layer, and layers 2 to L -1 are hidden layers. Let the number of neurons in the lth layer be $N_l, l = 1, 2, 3 \ldots \ldots, L$. Let w_{ij} represent the weight of the link between the jth neuron of the $l-1$th layer and the ith neuron of he lth layer. Let x_i represent the ith external input to the MLP and z_i be the output of the th neuron of the th layer. There is an additional weight parameter for each neuron (w_{i0}^l) representing the bias for the ith neuron of the lth layer. As such, of the MLP includes $w_{ij}^l, j = 0, 1, 2, \ldots \ldots . N_{l-1}, i = 1, 2, 3, N_l \;\; and\; l = 2, 3, \ldots . L, i.e.; w = \left[w_{10}^2\, w_{11}^2 w_{12}^2 \ldots \ldots w_{N_l N_{L-1}}^2\right]^T$

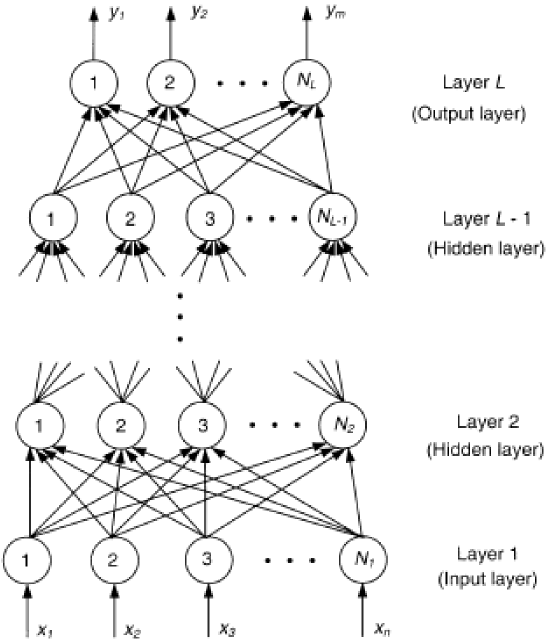

Fig. 4-3 MLP ANN structure [80]

The weight parameters are real numbers and initialized before training. During training, they are changed (updated) iteratively in a systematic manner. Once the training is completed, the vector remains fixed.

In the MLP network, each neuron processes the inputs received from other neurons. The input is processed by a function called the activation function in the neuron and output is transferred to the other connected neurons. As an example, every neuron in the l th layer receives input from the neurons of the $(l-1)$th layer, i.e., z_l^{l-1} z_2^{l-1} , …, $z_{N_{l-1}}^{l-1}$ A typical lth neuron in the lth layer multiplies the input by the corresponding weight parameter and then adds the products to produce a weighted sum γ_i^l.

$$\gamma_i^l = \sum_{j=0}^{N_{l-1}} w_{ij}^l z_j^{l-1} \quad (4.2)$$

To create bias, which is done by the parameter w_{i0}^l, a fictitious neuron in the $(l-1$)th layer whose output is $z_0^{l-1} = 1$ is assumed to exist. The weighted sum is used to activate the neuron's activation function to produce the final output of the neuron $z_i^l = 1$. This output will be the input to neurons in the $(l+1$)th layer. There are several activation functions such as sigmoid, arc-tangent, hyperbolic-tangent function, etc. All these are smooth switch functions that are bounded, continuous, monotonic, and continuously differentiable. The most commonly used hidden layer neuron activation function is the sigmoid function which is given by:

$$\sigma(\gamma) = \frac{1}{(1 + e^{-\gamma})} \tag{4.3}$$

Input neurons use a relay activation function and simply relay the external input to the hidden layer neurons, i.e $z_i^1 = x_i, i = 1,2,3, \ldots n$. In the case of obtaining neural networks for EM applications, where the purpose is to model continuous electrical parameters, a linear activation function can be used for output neurons. An output neuron computation is given by

$$\sigma(\gamma_i^L) = \gamma_i^L = \sum_{j=0}^{N_{L-1}} w_{ij}^L Z_J^{L-1} \tag{4.4}$$

Given the inputs and the weights, feed forward computation is a process used to compute the outputs. Feed forward computation is used both during neural-network training and during the usage of the resulted model. Firstly, external inputs are fed into first layer and the outputs from the input layer are fed to the hidden neurons of the second layer. Following this pattern, the outputs of the $L - 1$th layer are fed to the output layer (i.e., the L th layer). During feed forward computation, ANN weights **w** remain fixed. The feed forward computation is given by:

$$\begin{aligned} z_i^l &= x_{i,} \quad i = 1,2,3, \ldots \ldots \ldots \ldots \ldots, N_{1,} \, n = N_1 \\ z_i^l &= \sigma\left(\sum_{j=0}^{N_{l-1}} w_{ij}^l z_j^{l-1}\right), i = 1, 2, 3, \ldots \ldots \ldots \ldots \ldots .. N_l; \\ & \qquad l = 2,3 \ldots \ldots \ldots \ldots \ldots \ldots L. \\ y_i &= z_i^L \;\; i = 1, 2, \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \; N_L \;\; m \\ & \qquad = N_L \end{aligned} \tag{4.5}$$

ANN's weight parameters (**w**) are initialized to provide a good starting point for training which is done thru optimization. The widely used strategy for MLP weight initialization is to initialize the weights with small random values (e.g., in the range [-0.5, 0.5]).

The training data consists of sample pairs $\{(x_k d_k)\ and\ k \epsilon\ T_r\ \}$ where x_k and d_k are vectors representing the inputs and desired outputs of the neural network. We define neural-network training error as:

$$\sum_{T_r}(\boldsymbol{w}) = \frac{\mathbf{1}}{2} \sum_{k \epsilon T_r} \sum_{j=1}^{m} \left| y_j(x_{k,} w) - d_{jk} \right|^2 \qquad (4.6)$$

Where is $d_{jk}$the jth element of d_k and $d_{jk}$is the jth neural-network output for input x_k.The purpose of neural-network training is to minimize the error function $E_{Tr}(w)$.

Since $E_{Tr}(w)$ is a nonlinear function of the weight parameters **w**, iterative algorithms are often used to explore the **w**-space. Optimization algorithm starts with a initial value of **w** and then iteratively updates it. Gradient-based optimization algorithms update **w** based on error information$E_{Tr}(w)$ and error gradient information$\frac{dE_{Tr}(w)}{dw}$. The next point in **w**-space is determined by a step down from the current point along a search direction vector **h**, i.e. $\mathrm{w}_{\mathrm{next}} = \mathrm{w}_{\mathrm{now}} + \boldsymbol{\eta} h$. Here, $\Delta w = \boldsymbol{\eta} h$ is called the weight update also known as the learning rate. For example, the back propagation (BP) training algorithm updates **w** along the negative direction of the gradient of training error as **w** = $\mathbf{w} - \boldsymbol{\eta}(\frac{dE_{Tr}(w)}{dw})$.

A block diagram representation of the ANN training algorithm can be found in Fig. 4.4.

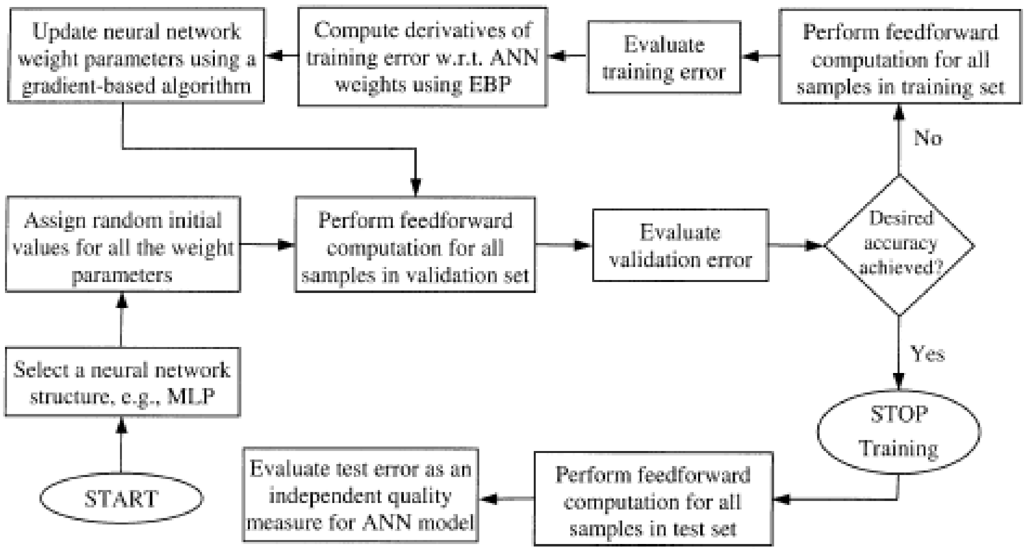

Fig. 4-4 Flowchart of ANN Training[80]

4.2.1.1 Modeling Results with ANN

In our study, 3 layered MLP structure and 300 epochs are used. Initial weights are chosen to be in a range of [-0.8 - 0.8]. As transfer functions, hyperbolic tangent sigmoid transfer function and linear transfer functions are used. Genetic algorithms are used for the optimizing the weights to minimize the model error. For this purpose Matlab GADS is used. Population size and maximum generations are determined to be 10. Crossover fraction is chosen to be 0.7 and eliteCount is chosen as 1. StallGenLimit value is 4 and StallTimeLimit is unbounded. Mutation is employed in GAs. More information about these options can be found in Matlab GADS documentation.

3 layers with 300 neurons ANN is employed in this study. As learning rules, Bayesian regulation backpropagation (trainbr), Levenberg-Marquardt backpropagation (trainlm) and scaled conjugate gradient backpropagation(trainscg) are used. 80% percent of samples are used for training, and remaining 20% are used for validation. The error measure is defined as root relative square error (RRSE) which is calculated by (4.1). Error measure is set to 0.1. ANN is found out to be the best modeler in our comparative study based on capturing the nonlinear behavior of the antenna but lacks speed. Choosing frequency and permittivity as the design variables, use of ANN with parameter settings above resulted in the surface in Figue 4.5.

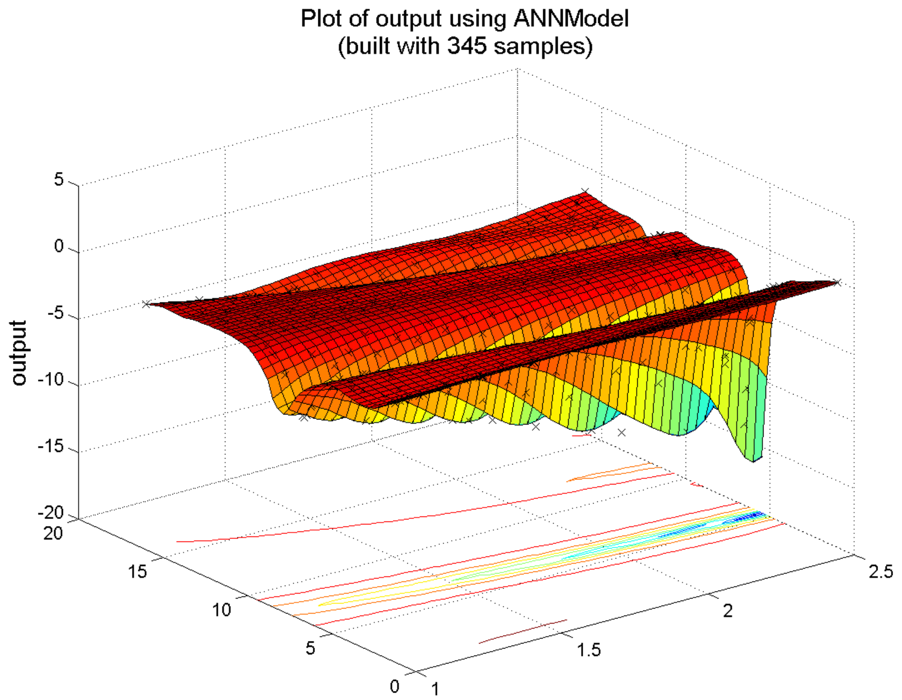

Fig. 4-5 Result of ANN modeling with 2 variables.

After obtaining satisfying surrogate modeling results, to explore the dependence of the framework and surrogate based models we increased the complexity of our model. In this study we ANN modeling in a domain consisting of 3 variables was peformed. Chosen variables correspond to permittivities of both layers supporting the patch antenna shown in Fig. 4.6, and its operating frequency. The parameter settings were successful due to the models capability in capturing the resonance trend. The model captured the resonance in 4 dimensional space (Fig 4.7), however model`s error measure did not converge to 0.1 value in feasible time. Due to some computational resource problems, the model simulations had to be stopped prematurely before reaching convergence.

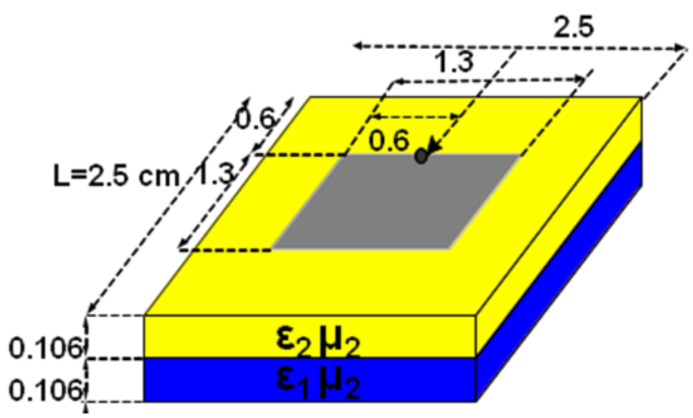

Fig. 4.6 Two layer patch antenna

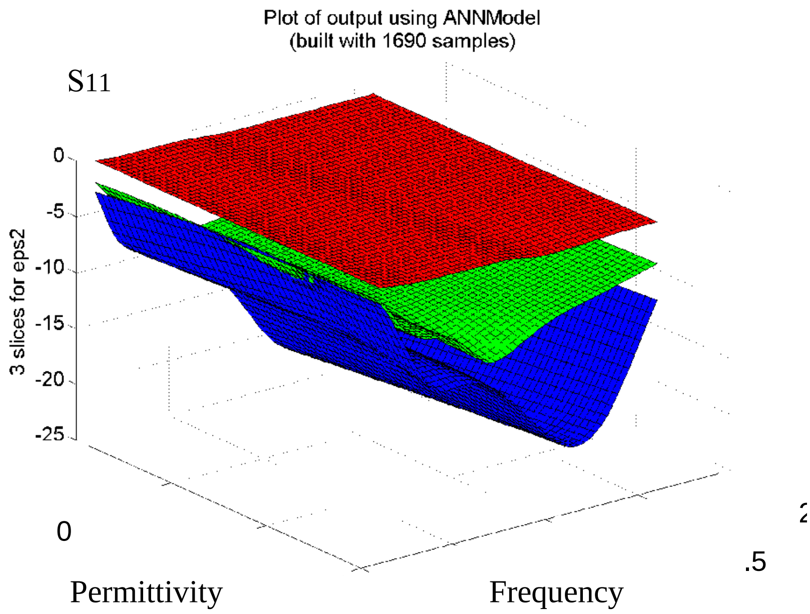

Fig. 4.7 ANN modeling with three variables

4.2.2 Kriging

Kriging is a method of curve fitting that was first reported in 1951 during mine searching for gold in South Africa by D.G. Krige. That system is mainly based on prediction a data point when the values around the data are known. During the 80's this topic again received attention from statisticians interested in creating effective metamodels for computer experiments [76]. The method then took form as a popular technique called Design and Analysis of Computer Experiments (DACE).

Most of the other metamodeling routines are based on the assumption that the metamodel is of the specific form: $y = f(x) + \in$. where $f(x)$ is the the assumed basis function and $\in$ is IID Gaussian random error with mean zero. Kriging does not make this assumption. In kriging, $\in$ is a function of x and the driver of kriging algorithm is this error measure. So the general form of kriging metamodel is as follows:

$$y(\boldsymbol{x}) = \boldsymbol{\beta}^T f(\boldsymbol{x}) + z(\boldsymbol{x}) \qquad (4.7)$$

Where $\boldsymbol{f} = [f_1(x) \quad \ldots \quad f_n(x)]^T$and $\boldsymbol{\beta} = [\beta_1 \quad \ldots \quad \beta_k]^T$

The matrix $\boldsymbol{f}$ corresponds to the various terms in the polynomial (including cross terms) and denotes the regression parameters. The term $z(\boldsymbol{x})$ refers to the functional departure of the predictor from the mean $\boldsymbol{\beta}^T f(\boldsymbol{x})$with the following properties which are given as:

$$E[z(\boldsymbol{x})] = 0$$

$$Cov[z(\boldsymbol{x}), z(\boldsymbol{w})] = \sigma_z^2 \, R(\boldsymbol{x}, \boldsymbol{w})$$

$$R = \begin{bmatrix} R_{11} & \ldots & R_{1n} \\ \vdots & \ddots & \vdots \\ R_{n1} & \ldots & R_{nn} \end{bmatrix} \tag{4.8}$$

$$R_{ij} = R(x_i, x_j) = \prod_{k=1}^{d} exp\left\{-\theta^k \left|x_i - x_j\right|^{p^k}\right\}$$

where R is the Spatial Correlation Factor matrix. The product correlation rule for R is the most widely used form of the covariance matrix [76]. Here, Gaussian correlation function is used. The parameters and $0 < \theta,\ 0 \leq p \ \leq 2$ determine the level of correlation and the smoothness of the correlating functions. One important characteristic of R is that $R(x, x) = 1$ and all other terms are between 0 (when the points are far apart) and 1(when the points are equal).

Let`s define the form of the kriging predictor. The $n \times 1$ correlation vector $\boldsymbol{r}$ and functional matrix be defined as follows:

$$\boldsymbol{r}(x) = [R(\boldsymbol{x_1}, \boldsymbol{x}) \quad R(\boldsymbol{x_2}, \boldsymbol{x}) \quad \ldots \quad R(\boldsymbol{x_n}, \boldsymbol{x})]^T$$

$$F = \begin{bmatrix} \boldsymbol{f^T}(\boldsymbol{x_1}) \\ \vdots \\ \boldsymbol{f^T}(\boldsymbol{x_n}) \end{bmatrix} \tag{4.9}$$

Where. $\boldsymbol{x}$ is any point in the domain and n is the number of sampled points. The objective is to find the best set of parameters that define the Best Linear Unbiased Predictor (BLUP) for the main function by minimizing the expected value
of squared error across the domain. This simply turns out to be a constrained convex optimization problem which can be solved with Lagrangian relaxation method [77].

The BLUP is the form $y(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x})^T S$ .where c is a vector function of x defining the predictor`s behavior. BLUP is found by minimizing the expected value of error given by $E(\boldsymbol{c}(\boldsymbol{x})^T S - y(x))^2$. Assuming the predictor is unbiased i.e $F^T c_x = f(x)$, the problem is simplified to:

$$\begin{aligned} \text{Minimize } & (\boldsymbol{c}(\boldsymbol{x})^T \sigma_z^2 R) c(x) + \sigma_z^2 - 2\boldsymbol{c}(\boldsymbol{x})^T \sigma_z^2 r \\ & - \lambda [F^T \boldsymbol{c}(\boldsymbol{x})^T - f(x)] \end{aligned} \tag{4.10}$$

By taking partial derivatives w.r.t $\boldsymbol{c}(\boldsymbol{x})^T$ and the Lagrange multipliers, λ, the solution is then reduced to solving a system of linear equations:

$$\boldsymbol{K} \begin{bmatrix} -\lambda \\ c_x \end{bmatrix} = \begin{bmatrix} -\boldsymbol{f}(\boldsymbol{x}) \\ \sigma_z^2 \, \boldsymbol{r}(\boldsymbol{x}) \end{bmatrix}, \text{ where } K = \begin{bmatrix} 0 & \boldsymbol{F}^T \\ \boldsymbol{F} & \sigma_z^2 \, \boldsymbol{R} \end{bmatrix} \tag{4.11}$$

, where
And the final form of the BLUP is given by

$$y(x) = f^T(x)\boldsymbol{\beta} + \boldsymbol{r}^{\boldsymbol{T}}(\boldsymbol{x})\boldsymbol{R}^{-\boldsymbol{1}} (\boldsymbol{S} - \boldsymbol{F}^{\boldsymbol{T}}\boldsymbol{\beta}) \tag{4.12}$$

Where $\boldsymbol{\beta} = (\boldsymbol{F}^T \boldsymbol{R}^{-\boldsymbol{1}} \boldsymbol{F})^{-\boldsymbol{1}} \boldsymbol{F}^T \boldsymbol{R}^{-\boldsymbol{1}} \boldsymbol{S}$

The variance of the predictor is given by:

$$\begin{aligned} \sigma_y^2(\boldsymbol{x}) = \sigma_z^2 & \left\{ 1 - [\boldsymbol{f}^{\boldsymbol{T}}(x) \quad \boldsymbol{r}^{\boldsymbol{T}}(\boldsymbol{x})\ ] K^{-1} \begin{bmatrix} \boldsymbol{f}^{\boldsymbol{T}}(\boldsymbol{x}) \\ \boldsymbol{r}(\boldsymbol{x}) \end{bmatrix} \right\} \\ & \approx \sigma_z^2 (1 - \boldsymbol{r}^{\boldsymbol{T}}(\boldsymbol{x})\boldsymbol{R}^{-\boldsymbol{1}} \boldsymbol{r}(\boldsymbol{x})) \end{aligned} \tag{4.13}$$

The form of the predictor is developed above, and now the parameters need to be determined. Parameters p and θ are found using maximum likelihood method. This problem is in the below form:

$$\text{Maximize } -\frac{1}{2}[n \ln(\sigma_z^2) + \ln \det(R)]$$
$$\text{Subject to: } 0 < \theta,\ 0 \le p \le 2 \tag{4.14}$$

This form turns out to be a constrained convex optimization problem which can be solved using SQP, intrior point solvers or heuristic methods such as GAs.

4.2.2.1 Modeling Results with Kriging

In the sumo toolbox that was used during the simulation process spline, exponential, linear and Gaussian correlation functions were available to use. Our simulations used mostly the Gaussian one which has a more common usage compared to the others. The fitted kriging metamodel is given in Fig. 4.8. As Matlab kriging options, regpoly1 is used for regression Function and corrgauss is used as correlation function. Lower theta bound is -5 and upper bound is 3. Polynomial regression is chosen and Gaussian correlation is used in this work. Model hyper-parameters are found by genetic algorithms. Population size and maximum generations is determined to be 10. As population type doubleVector is used. Elite count value is 1, Crossover fraction is 0.7, stallGenLimit value is 4 and StallTimeLimit value is infinity. As crossover function heuristic method is used. More information about these options can be found in Matlab GADS documentation.

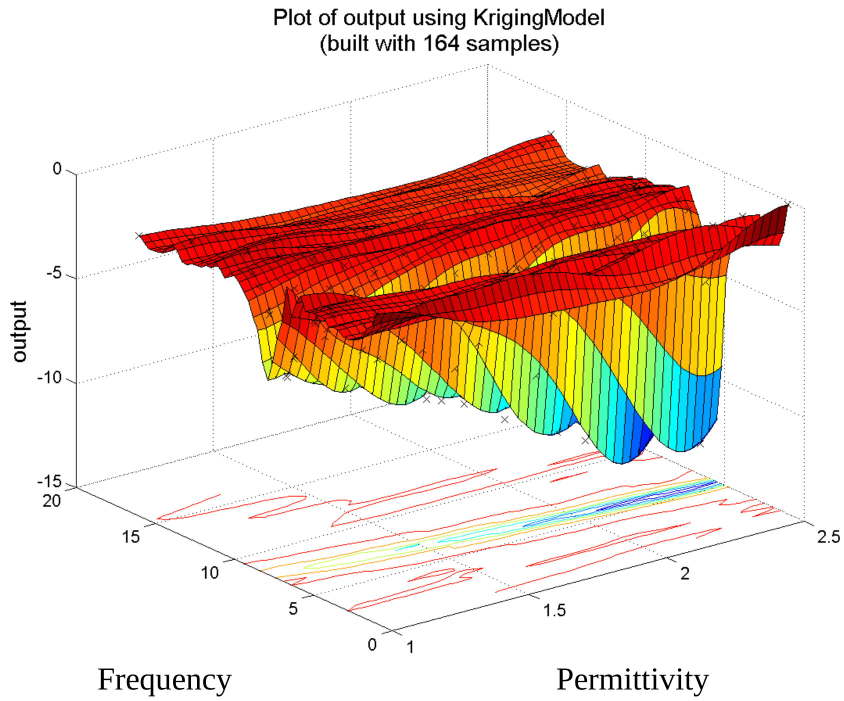

Fig. 4.8 Modeling Result with Kriging

4.2.3 Radial Basis Functions (RBF)

A radial basis approximation takes the form:

$$\boldsymbol{S}(\boldsymbol{x}) = \sum\nolimits_{\boldsymbol{i}\,\in \boldsymbol{I}} \boldsymbol{y_i}\, \boldsymbol{\sigma}(\| \boldsymbol{x} - \boldsymbol{i} \|), \quad \boldsymbol{x} \in \boldsymbol{R^d} \tag{4.15}$$

Where $\varphi: [0, \infty) \rightarrow$ R is a fixed univariate function and the coefficients $(\mathrm{y_i})_{i\epsilon I}$ are real numbers.

The weighted multiples also can be chosen following different strategies. One of them is an iterative process that is known linear least squares, which is a method of fitting a curve from known values by minimizing the distance to the fitted curve. GA is used in our studies to determine the weights.

RBF basis functions:

- Gaussian

$$\sigma(r) = \exp(-\beta r^2),\ \text{For some } \beta > 0 \tag{4.16}$$

- Multiquadratic

$$\sigma(r) = \sqrt{r^2 + \beta^2},\ \text{For some } \beta > 0 \tag{4.17}$$

- Polyharmonic spline:

$$\sigma(r) = r^k, k = 1,3,5 \ldots. \tag{4.18}$$

Thin plate spline (a special polyharmonic spline)

$$\sigma(r) = r^2 \ln r \tag{4.19}$$

4.2.3.1 Modeling Results with RBF

For the hyperparameter estimation GAs has been used. Population size is chosed to be 15. Crossover Fraction value is 0.7, Maximum generation number is 10, and Elite Count is 1. Mutation is allowed in the population. More information about these options can be found in Malab GADS toolbox documentation

Bounds for the shape parameters for basis functions such as Gaussian function, multiquadratic function and exponential function are between 0.1 and 5 in logarithmic scale.

Modeling results are satisfactory and shown is Fig. 4.9, run is faster than ANN however RBF is more sensitive to sample distribution over domain which means the tendency of resulting in different models for different runs with different samples is higher.

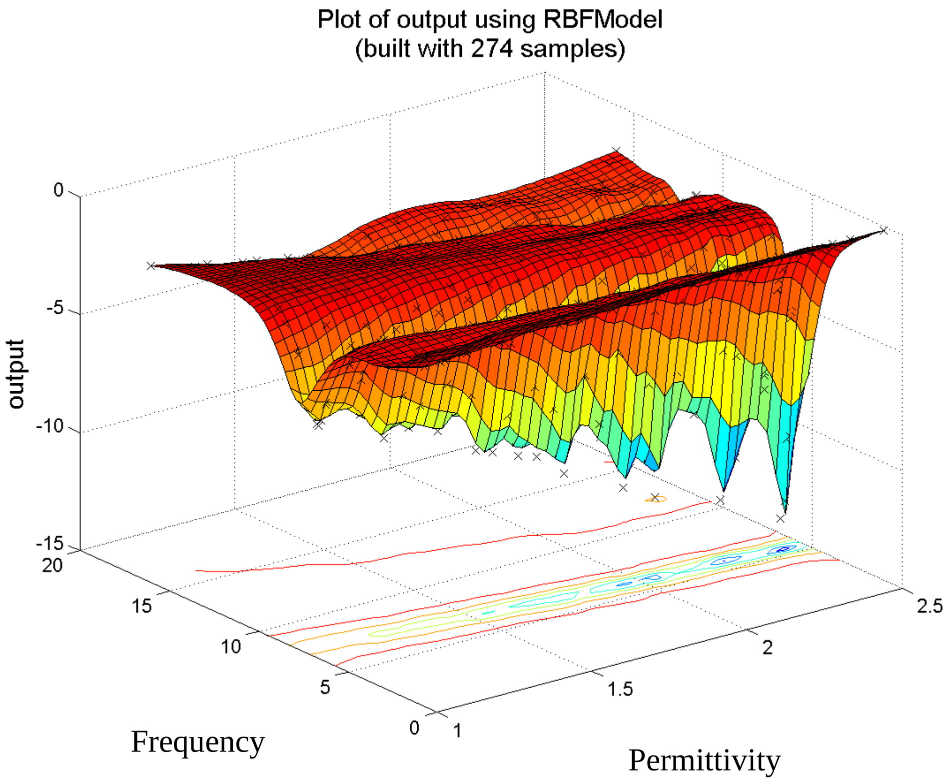

Fig. 4.9 Result of modeling with RBF

4.2.4 Support Vectors Machines (SVM)

Support Vector Machines is a system of data fitting, prediction that is based on statistical learning theory which is a machine learning method. Statistical Learning Theory is based on making predictions about the data, observing the results and making new guesses based on these results. [69]

Support Vector Machine can find the optimal hyper plane that is bound to some constraints. Finding the optimal plane problem can be reduced to a dual problem using Lagrange Optimal Methods, which can be represented as:

$$Max\ Q(\alpha) = \sum_{1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \left(x_i x_j\right) \tag{4.19}$$

Where α_i is the Lagrange Multipliers, When the problem above is solved the optimal classification is obtained as follows:

$$f(x) = sgn\big((wx) + b\big) = sgn\{\sum_{i=1}^{n} \alpha_i y_i (x_i x) + b\} \tag{4.20}$$

Here if the Kernel function of the domain is used the inner product in the first problem ($x_i x_j$) can be replaced by $K(x_i x_j)$ and the problem can be rewritten as:

$$Max\ Q(\alpha) = \sum_{1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j\, K\big(x_i x_j\big) \tag{4.21}$$

And the optimal classification can be rewritten as:

$$f(x) = sgn\big((wx) + b\big) = sgn\{\sum_{i=1}^{n} \alpha_i y_i K(x_i x) + b\} \tag{4.22}$$

In this case the problem is reduced to linearly separable cases and the machine which does this process is called the SVM

4.2.4.1 Modeling Results with SVM

Kernel Parameter bounds are chosen to be in the range of [-4,4]. Regression Parameter bounds are [-5,5]. Nu is chosen 0.01. SVM is slower than RBF but faster than ANN. It is less sensitive than kriging to sample distribution. Hyper-parameters are found with GAs. For this purpose Matlab GADS is used. Population size and maximum generations are determined to be 10. Crossover fraction is chosen to be 0.7 and eliteCount is chosen as 1. StallGenLimit value is 4 and StallTimeLimit is unbounded. Mutation is employed in GAs. More information about these options can be found in Matlab GADS documentation.

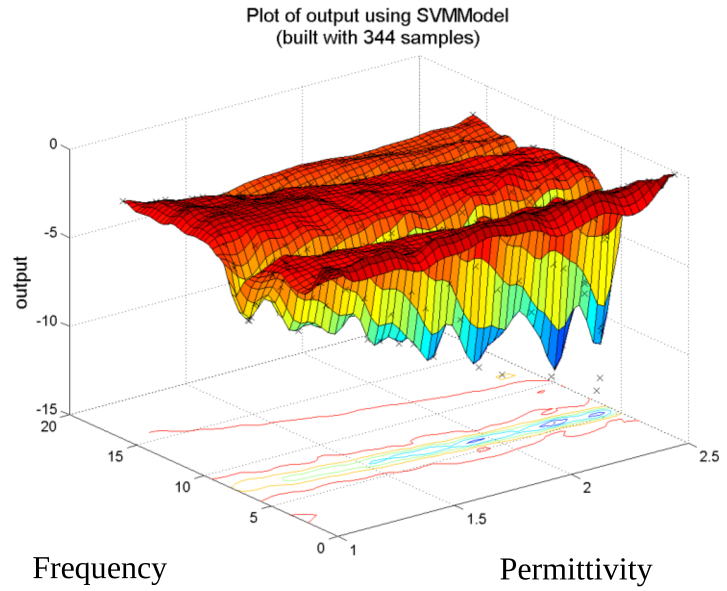

Fig. 4.10 Modeling with SVM

4.2.5 Rational Model

Rational functions are natural choices for modeling resonance behaviors of Electro-Magnetic devices since the input and outputs of these devices can be represented in the rational way based on the transfer function. A typical property of these rational functions is that they are both rational and orthogonal which means they can be written as the ratio two different polynomial functions. Orthogonal functions are generally can be shown as:

$$< f, g > = \int f^{*}(x).g(x)dx = 0 \qquad (4.23)$$

Here f^{*} is used to denote the complex conjugate of the functions.

Rational Model can be based on mainly three different well defined functions which are Power, Legendre and Chebyshev.

Legendre functions can be generally described as the solutions to the Legendre's differential equations.

$$\frac{\mathrm{d}\{(1 - \mathrm{x}^2 \frac{\mathrm{d}}{\mathrm{dx}} \mathrm{P_n(x)}\}}{\mathrm{d}} + \mathrm{n(n+1)P_n(x)} = 0 \qquad (4.24)$$

Here P_n can be described as:

$$(2n+1)P_n(x) = \frac{d}{dx}[P_{n+1} - P_{n-1}(x)] \quad (4.25)$$

Here it can be seen that the function is recursive, also generally the function is convergent to some value when limit is taken.

Chebyshev rational functions are another type of functions that are used as basis functions for rational genetic models. An example for that type of functions of degree n:

$$R_n(x) = T_n(\frac{x-1}{x+1}) \quad (4.26)$$

Here T_n denotes a Chebyshev function of first kind which can be represented in the recurrence relations:

$$\mathrm{T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)} \quad (4.27)$$

Here the function is again both rational and orthogonal as that was the case in the Legendre functions.

Using different basis functions and settings several runs have been done, but due to some problems with fitting algorithm, results are not presented here.

5 SURROGATE MODEL ASSISTED MULTI-OBJECTIVE DESIGN OPTIMIZATION-A PRELIMINARY STUDY

5.1 Surrogate Model Based Design Optimization Framework

Addressing large scale design optimization problems in a feasible time using costly simulations for analysis is almost impossible. There are two ways to face this challenge: 1. Naïve way is to increase the computational power limited by available computational resources, and 2. Alternatively, to solve the problem by making re-analysis faster. The main time consuming component of the design optimization framework is the computational analysis tool. Surrogate models are fast-running approximate substitutes of complex and time-consuming computer simulations of the exact model. They capture the complex behavior of the underlying simulation model and they are model-specific. Thus, integration of fast surrogate models into our design optimization framework should allow for the solution of challenging EM design problems (Fig 5.1).

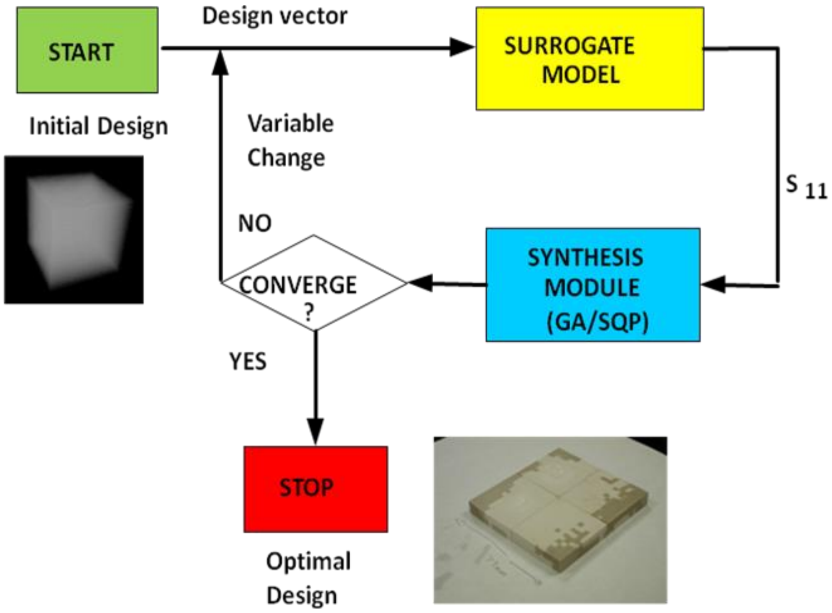

Fig. 5-1 Integration of Surrogate Models into Design Optimization Framework

The integrated design optimization framework is based on using hybrid design optimization techniques with various surrogate modeling tools towards the goal of designing volumetric material and conductor variations of complex electromagnetic devices. The framework should allow from scratch identification of the novel device structure, both its material and conductor variation in three dimensions, in an automated and efficient manner subject to some performance and size constraints. For the synthesis module, gradient-based optimizers such as Sequential Quadratic Programming (SQP) and global optimizers such as Genetic Algorithms are both utilized to allow for known advantages in terms of speed and global search capability, respectively. As the analysis module, two full wave electromagnetic wave solvers, i.e. a commercial EM simulator, Ansoft HFSS, and an in-house hybrid FE-BI based analysis tool are utilized. The design framework is primarily based on interfacing the analysis tools with various surrogate based models and linking it to the optimization tools.

5.2 Design Example 1: ANN model assisted Patch Antenna optimization

5.2.1 Design Model and Surrogate Model Parameters

Artificial Neural Networks was the most efficient and accurate surrogate model among various techniques presented in chapter 3, hence ANN is used as the surrogate model in this example. The design model of the chosen patch antenna is depicted in Fig. 5.2.

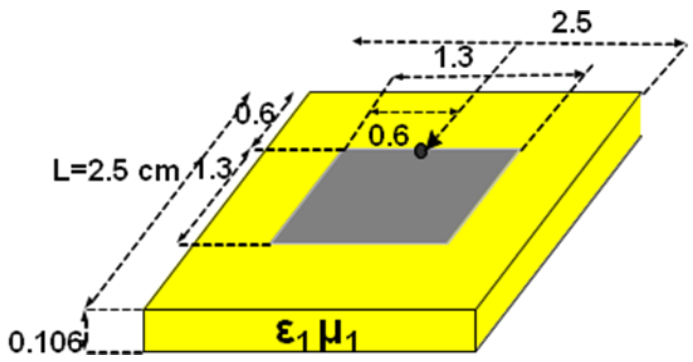

Fig. 5-2 Design Model of Patch Antenna

The permittivity of the layer is selected as the design variable [1-21] to investigate dielectric material effects on the performance. HFSS is capable of simulating the electromagnetic response of the device. The Frequency range of operation is specified as [0.7-9] GHz. The Latin Hypercube Method is used as the Design of Experiments (DOE) scheme as the sampling strategy. For the purpose of generating surrogate models, SUMO is integrated with our automated design platform within a MATLAB interface. In addition to the DOE scheme, adaptive sampling which is based on the combination of the accuracy of the model and density of the samples over the design domain is used with the goal of producing models with improved quality provided by SUMO. As a model validation metric, validation set with 80% of sampling used for training and 20% of sampling used for validation is chosen for its efficiency. The error measure is defined as RRSE. Error measure is set to 0.1 proven to be 'good quality' measure based on some trial and error runs. With the above mentioned surrogate model parameters, first surrogate model in Fig. 5.3 is obtained for the return loss response. This model is then used as the analysis tool within the integrated design optimization framework.

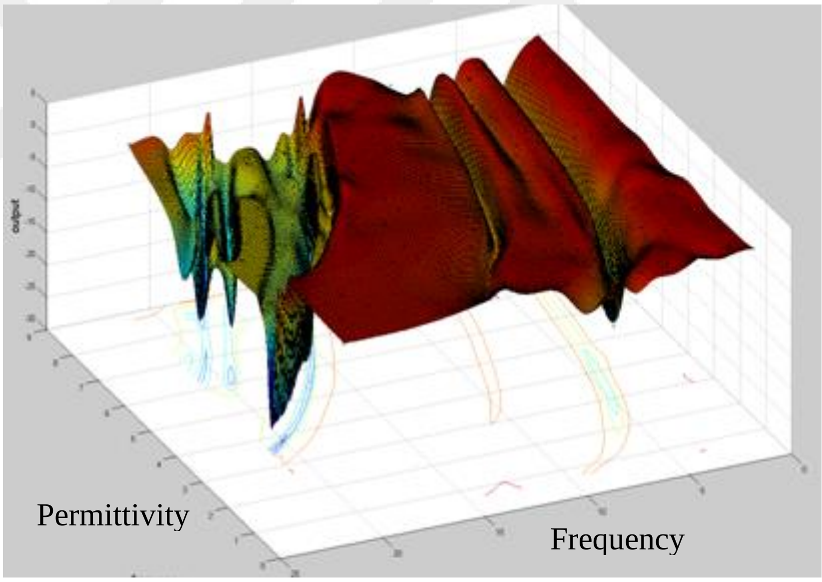

Fig. 5-3 ANN Model of Design Example in Fig. 4.2

For optimization purposes, GA is chosen for the global optimum search of the permittivity of the substrate. Population size is chosen to be 10 and maximum generations are set to 100. Mutation function is chosen as Gaussian which has a mean of value 1 and its variance is -0.3. Crossover function option is chosen to be "intermediate". Tournament selection function is employed.

5.3 Design Results

Based on the convergence history and the design results for the best individual value with ε=15 shown in Fig. 5,4, the ANN surrogate model integrated design optimization framework is successful. Based on a comparison with standard optimization effort without surrogate models, ANN-GA assisted design leads to 80% CPU time savings. More specifically, standard optimization with calls to the exact finite element based analysis code takes 116 hours to converge while surrogate model assisted design optimization takes about 23 hours on a Dell Intel(R) Exon(TM) 3.2 GHz CPU with 8 GB RAM.

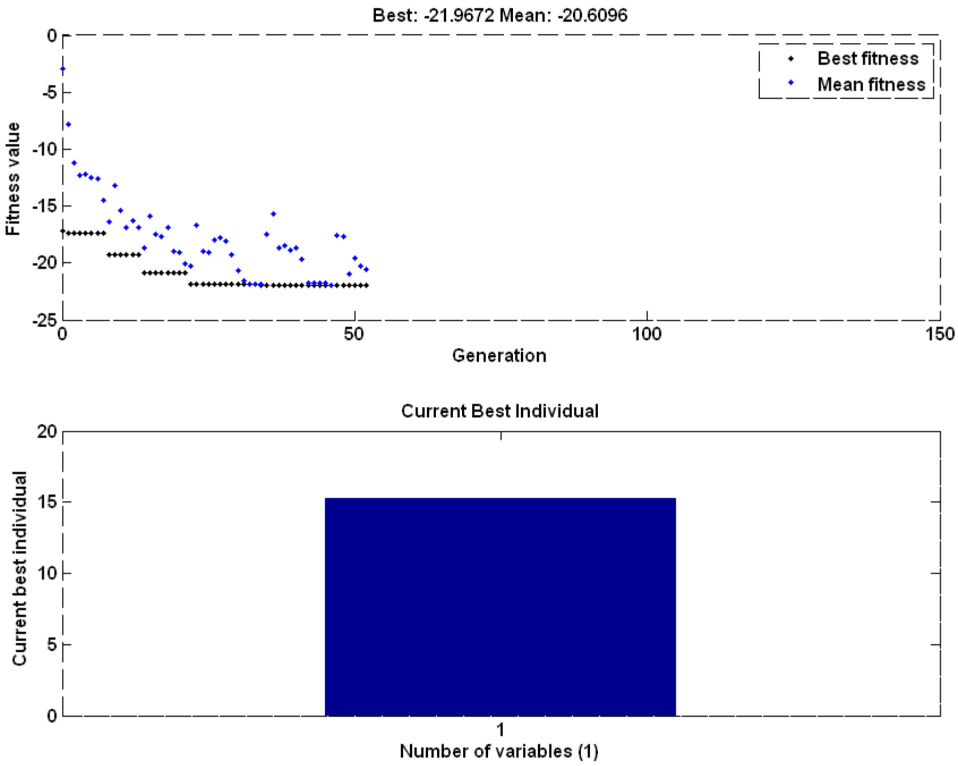

Fig. 5-4 GA Optimization History and Best Individual Value

Detailed time calculations are done for both cases. Standard optimization (with calls to original analysis code) takes 116 hours (Time = 100 generation * 10 individual * 7 min (per frequency sweep) = 7000 min = 116 hours). ANN Surrogate model assisted optimization takes 23 hours (Time =700 samples *2 min (per single frequency) = 1400 min = 23 hours). It is seen that ANN-GA assisted design saves 80% CPU time.

5.4 Multi-Objective Optimization Framework

Most real world problems are multi-objective in nature. They have several possibly conflicting objectives to be satisfied at the same time. In this situation, instead of aiming a single 'best' solution, optimization efforts concentrate on generating a set of good solutions which incorporate the trade-offs of the objectives and design decision maker can choose the solution based on his/her needs [71].

Multi-objective optimization more formally can be explained as follows [70]:

A vector of decision variables which satisfies constraints and optimizes a *vector function* whose elements represent the objective functions. These functions form a mathematical description of performance criteria which are usually in conflict with each other. Hence, the term "optimizes" means finding such a solution which would give the values of all the objective functions acceptable to the designer.

In mathematical form:

$$\begin{gathered} \min\,(f) \\ min[f_1 \quad f_2 \quad \dots. \quad f_n]^T \\ \text{s.t.} \\ g(x) \leq 0 \\ h(x) = 0 \\ x_l < x < x_u \end{gathered} \tag{5.1}$$

Where f_i is the *i*-th objective function, *g* and *h* are the inequality and equality constraints, respectively, and *x* is the vector of design variables. The solution to the above problem is a set of Pareto points. Pareto solutions are those for which improvement in one objective can not occur without worsening of at least one other objective. In traditional mathematical programming, we have one optimal solution whereas in multi-objective optimization framework, there could be numerous solutions and the curve of solution points is called the "Pareto Curve".

A design point in objective space spanned by each objectives, f^* is termed Pareto Optimal, if another feasible design objective vector f does not exist such that $f_i \leq f_i^*$ for all $i\epsilon\{1,2,\dots,n\}$ and $f_j \leq f_j^*$for at least one index of $j\epsilon\{1,2,\dots,n\}$.

Several solution methods have been proposed for the above problem in literature: Normal Boundary Intersection (NBI) method, construction of a single aggregate objective function (AOF), Normal Constraint (NC) method, Multi-objective Optimization Evolutionary Algorithms (MOEA), and PGEN (Pareto surface generation for convex multi-objective instances) are some well known strategies. In our work, we will integrate NBI within our design optimization framework for its known advantage of providing the designer with equally spaced Pareto solutions as a result of an easily adopted efficient search algorithm. Short description of the method is given next.

5.4.1 Normal Boundary Intersection (NBI) Method

The normal-boundary intersection method uses a geometrically intuitive method to produce an even spread of points on the Pareto surface applicable for all dimensions. NBI can be combined with a Pareto filter to identify non-Pareto points on the boundaries of the feasible region. NBI starts with finding the extreme values of each individual objective. Then other points on the Pareto surface are found by solving a sequence of single objective optimization problems. If the single objective problems are solved with a gradient based optimization method such as SQP then we also need derivatives. Gradients for complex systems such as patch antennas unless the analysis code is transparent are calculated mostly with finite differences which will require running vast amount of computer simulations for each variable. Also, the sub-problem solutions would depend on initial points which might not result in the global optimum. Heuristic methods such as GAs would as well require lots of costly simulations for the sake of an effective design space coverage. This process is computationally very costly. Hence a simple application of the NBI method via local optimization tools such as MATLAB's SQP is used in this work for the advantage of fast convergence.

5.4.2 Surrogate based Pre-Analysis Results

Our design efforts of patch antennas target large bandwidth and high gain performance. For initial testing of the framework, the patch antenna model in Fig. 4.2 is considered. The permittivity is chosen as a design variable and its range is determined to be within the bounds of [1-16]. Frequency range is specified to be between [1- 2.5] GHz, a common telecommunication frequency range. For surrogate modeling of the bandwidth of the patch antenna, ANN is used. GA is chosen for the hyper-parameter tuning of ANN model. Latin hypercube design is employed for design of experiments (DOE) scheme. For building the surrogate model of the gain performance, Radial Basis Functions are chosen with the DOE and the same hyper-parameter settings as in the ANN assisted return loss model. An HFSS script serving as the interface of the integrated framework is written for the patch antenna design, then turned into a MATLAB function and integrated into Surrogate Modeling Toolbox (SUMO). Error norm is determined to be less than 1% as in earlier design cases. Surrogate models were constructed with 345 and 249 samples for return loss and gain and are shown in Fig. 5.5 and Fig. 5.6, respectively.

After obtaining accurate surrogate models, these are used to perform optimization with a GA to find each objectives functions’ global optimum. These values are then fed into the NBI as the maximum point. Afterwards, the search for equally spaced points on the Pareto surface are to be found by solving a sequence of single objective optimization problems with tools such as sequential quadratic programming aided by finite differencing. Since we have accurate surrogate models for gain and bandwidth, it is very easy to obtain the middle points of the Pareto surface. Although the NBI framework has set up and utilized in the design of multi objective metamodel assisted one layer patch antenna, the algorithm didn`t converge since there was no improvement in bandwidth due to the nature of well known physical property where only one layer effective material change does not affect bandwidth.

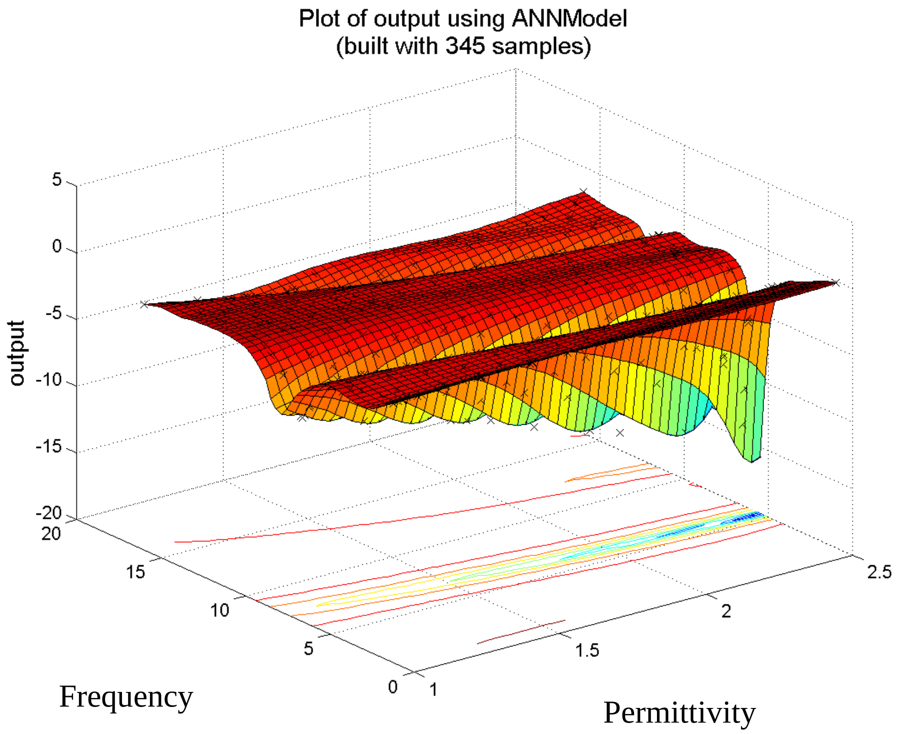

Fig. 5-5 Ann model of antenna return loss

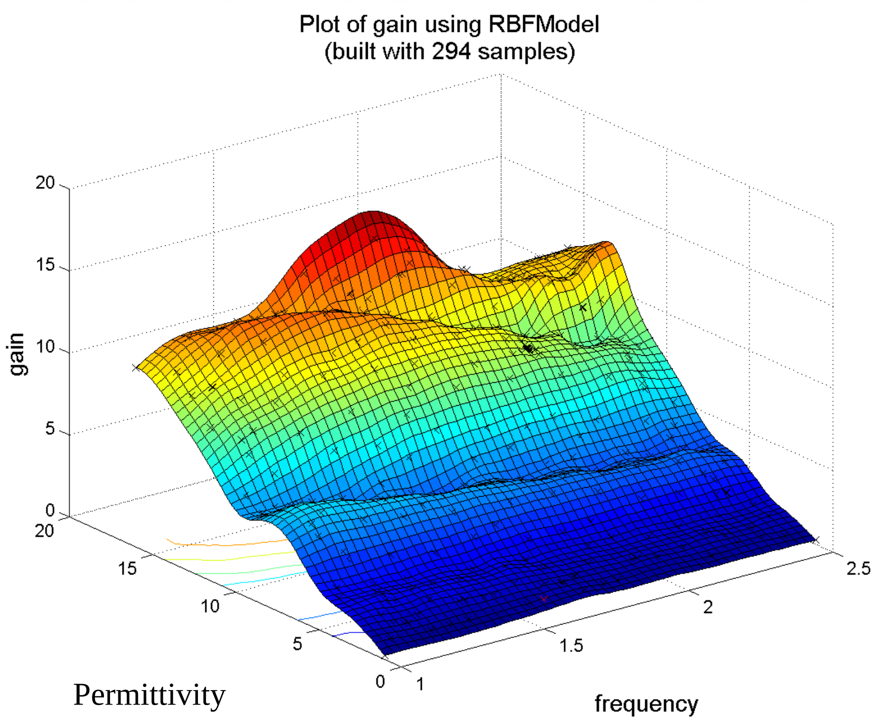

Fig. 5-6 RBF model of antenna gain

6 CONCLUSIONS AND FUTURE WORK

Formal design optimization can explore the ultimate optimal design in untouched design regions spanned by unknown degrees of freedom. However, large scale design optimization problems such as volumetric material explorations are computationally very expensive and demand high resources. To address this issue, in this thesis, we present an efficient design optimization framework for electromagnetic applications. The framework is based on integrating design optimization techniques with various surrogate modeling tools. The resulting framework is applied to the design of a micro-strip patch antenna using FSDA as analysis tool and SQP as synthesis tool. Considerable bandwidth improvement is achieved in working frequency range. Following this study, HFSS is integrated into optimization platform and the resulting framework is applied for the design of optical plasmonic nano-antenna. In this study, the interaction of light with plasmonic nano-antennas is investigated. An extensive study is performed to investigate the effect of the geometric and material properties of nano-antennas on the transmission efficiency. A modeling based automated design optimization framework is also developed. The results of the optimization framework are compared with those of the brute-force simulations. In these two design practices, it is observed that large scale design optimization problems took a large amount of time so that optimization study turned out being infeasible. To allow for considerable speed-ups of the versatile automated design process proposed here, automated and adaptive Design of Experiment (DOE) scheme is employed over the design domain and various surrogate models are compared within the design framework with respect to their performance. Multiple surrogate modeling techniques are investigated such as Artificial Neural Networks (ANN), Radial Basis Functions (RBF), Support Vector Machines (SVM) and Kriging. Results based on investigations show that ANN and RBF are more promising in terms of capturing the overall resonance behavior of the patch antenna when compared with Kriging and SVM. ANN is integrated into proposed design optimization framework. Results showed that the hybridized surrogate model based design framework allows for large number of design variables and suggests the effective and global exploration of the large-scale design space. Micro-strip patch antenna is optimized for bandwidth using surrogate model assisted design optimization framework. Based on a comparison with standard optimization effort without surrogate models, ANN-GA assisted design leads to 80% CPU time savings. Following this, a multi-objective surrogate model assisted design optimization framework is constructed and applied to the design of a patch antenna subject to maximum bandwidth and gain criteria. It is noted that this preliminary study focused on the substrate material effect on bandwidth and gain only for initial testing of the framework and easy interpretation purposes. However, bandwidth improvements of antennas, as is well known, are possible through other standard ways such as addition of radiating elements, material grating via layers with different magneto-dielectric properties, or resistive cards, modification of feed type and location and conductor shape and substrate thickness modifications. Their incorporation would naturally imply higher dimensionality of the design problem and surrogate model, hence, would call for larger computational resources and further investigations. Since the computational resources and time budget for this work were limited, this framework is applied to a simple one layer patch antenna example with a focus on the material substrate as the single variable. However, the framework due to its modular structure and flexible user interface should be capable of addressing other design problems with more degrees of freedom such as the 2-layer 3 variable surrogate model as investigated in Chapter 3. Major future work comprises further studies to apply this framework to design problems with more degrees of freedom and integrating this framework with inverse topology optimization problems addressing more challenging EM design problems giving rise to unique devices with increased design degrees of freedom.

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