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METAMODEL BASED ANALYSIS AND ITS APPLICATIONS: A REVIEW

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ABSTRACT: Engineering analysis using computer based simulation is used extensively to predict the performance of a system. Such engineering analyses rely on running expensive and complex computer codes. Approximation methods are widely used to reduce the computational burden of engineering analysis. Statistical techniques such as design of experiments and Response Surface Methodology (RSM) are widely used to construct approximate models of these costly analysis codes which minimize the computational expense of running computer analyze. These models referred as metamodels, are then used in place of the actual analysis codes to reduce the computational burden of engineering analyses. Use of metamodels in the design and analysis of computer experiments has progressed remarkably in the past three decades. This paper reviews the state of the art of constructing metamodels and its evolutions over the past three decades.
KEYWORDS: Metamodel, Experimental design, Approximation methods, Response surface, Kriging, Reliability based design

INTRODUCTION

Engineers use finite element analysis packages to evaluate the performance of a structure, computational fluid dynamics packages to predict the flow characteristics of a fluid media in or over a domain and Monte Carlo Simulation (MCS) to estimate the reliability of a product. Also traditional engineering design optimization which is the process of identifying the right combination of product parameters is often done manually, time consuming and involves a step by step approach. Approximation methods are widely used to reduce the computational burden of engineering analyses.

The use of long running computer simulations in design leads to a fundamental problem when trying to compare and contrast various competing options. It is also not possible to analyze all of the combinations of variables that one would wish. Metamodels, also referred as surrogate models, are a cheaper alternative to costly analysis tools and can significantly reduce the computational time involved. The basic approach is to construct a mathematical approximation of the expensive simulation code, which is then used in place of the original code to facilitate analysis such as design optimization, reliability analysis, etc.

A variety of approximation methods exists (e.g. response surface, kriging model, radial basis function, neural network, regression splines), and recently Simpson et al. [1] presented a general overview of how this area has been developed over the past two decades. Wang et al. [2] offers an overall picture of the current research and development in metamodel based design optimization. Simpson et al. [3] also reviews on metamodel based design optimization including several experimental design methods, RSM, Taguchi methods, neural networks, and kriging. Recommendations for the appropriate use of statistical approximation techniques were also given in the paper. A panel discussion on approximation methods in multidisciplinary analysis and optimization was held at the 9th AIAA/ISSMO Symposium on Multidisciplinary Analysis & Optimization in Atlanta during 2002.

The objective of the panel was to discuss the available approximation methods and identify the future research directions [4]. Forrester et al. [5] reviews a range of surrogate modeling methods, their use in optimization strategies and noted the pros and cons of each method. They have also provided some general thoughts on the suitability of each method for various types of problems.

Many review papers have been reported since three decades in the application of metamodel in design optimization. It also seems that more and more methods are being developed, the gap between research community and design engineers keeps widening.

This review is expected to provide the current research and development of metamodel based analysis. Moreover, it is organized in a way to provide the researcher's the application of metamodels in design optimization and reliability based design. Though efforts have been made to collect as much relevant literatures as possible, it is not the intent of the review to be exhaustive on this intensive topic.

ROLE OF METAMODELING

Detailed research has been carried out in using metamodeling techniques in design optimization. This research includes experimental design methods, metamodel types, model fitting techniques, application of metamodels in design optimization and reliability based design. Through literatures it has become clear that metamodeling provides a decision support role for all design engineers. The supporting functions that metamodels can provide are listed here with reference to the literatures [6]:

a) Model approximation-models which replace the computationally expensive codes,
b) Design space exploration-understanding the design problem in the whole design space by using metamodels,
c) Optimization – e.g., global optimization, multi-objective optimization, multidisciplinary optimization, probabilistic optimization and so on. Metamodels are integrated to the above optimization problems to reduce the computational burden.
d) Reliability based design- Reliability assessment is the prime function for Reliability based design. Metamodels are used to approximate the expensive constraint functions, or the limit state function.

Figure 1 illustrates the support afforded by metamodels.

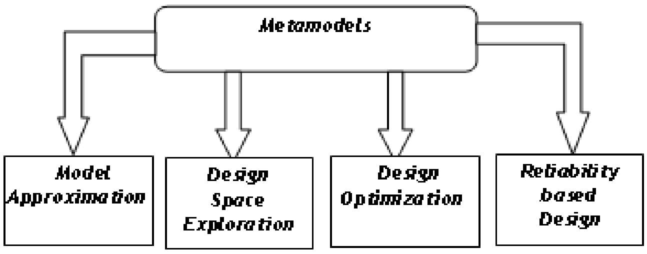


Figure 1. Support provided by metamodels

The evolution of metamodel based analysis is summarized in figure 2, which shows the number of publications related to metamodels over the past three decades. This data was obtained using the 'Scirus scientific research tool' where we searched for occurrences of the word: "metamodels"(during May 2011). Figure 3 illustrates the number of publications reporting the use of metamodels in design optimization and reliability analysis applications. For each application, the search was made with the following words: metamodels AND design optimization or metamodels AND reliability analysis.

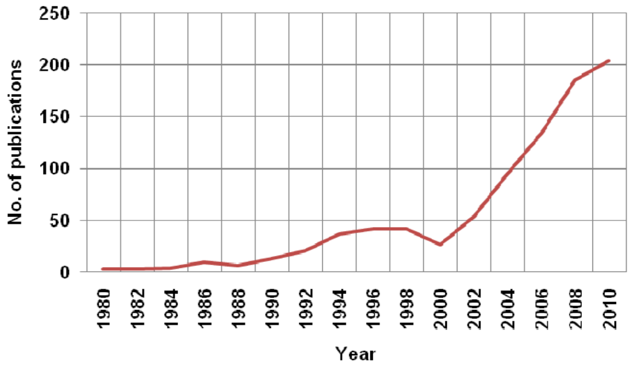


Figure 2. No. of publications, from 1980 - 2011

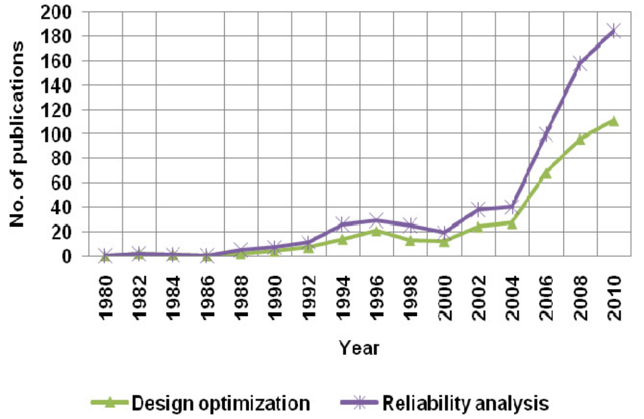


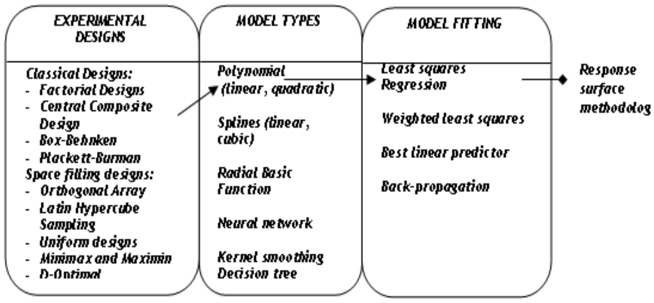
Figure 3. Metamodels in design optimization and reliability analysis

METAMODELING

Metamodeling involves (a) Selection of experimental design for generating data, (b) Selection of model to represent the data, and (c) fitting the observed data using the model. There are several options for each of these steps, as shown in figure 2. For example, response surface methodology usually employs central composite designs, polynomials and regression analysis.

Experimental designs

An experimental design (or Design of experiments) is an organized method to determine the relationship between the different factors affecting the output of a process. As indicated in Figure 4, there are several experimental design methods. Design of Experiments includes the design of all information-gathering exercises where variation is present, usually under the full control of the experimenter. Often the experimenter is interested in the effect of some process or intervention on some objects. Design of experiments is a discipline that has very broad application.



Figures 4. Types of Metamodelling Techniques

Classical design and analysis of physical experiments accounts the random variation by spreading the sample design points in the design space and by taking replicate design points. Commonly used classical designs are factorial or fractional factorial, Central Composite Design(CCD), Box-Behnken design, Plackett-Burman design. Also classical designs spread the sample points around the boundaries and leave a few at the center of the design space. Sacks, et al. [7] stated that as computer experiments involve mostly systematic error rather than random error, a good experimental design tends to fill the design space. They also stated that to classical designs, e.g. CCD can be inefficient or even inappropriate for deterministic computer codes. Jin, et al. [8] also confirms that experimental designs for deterministic *computer analysis should be space filling. Koehler and Owen [8] described several space filling designs like maximum entropy design, mean squared-error designs, minimax and maximin designs, Latin Hybercube designs, orthogonal arrays and scrambled nets. The most common space filling designs available in the literatures are Latin Hypercube [9-31], orthogonal arrays [18, 32-41], Hammersley sequences[42-50] and uniform designs[51,52]. The code for generating various designs is available at http://lib.stat.cmu.edu/designs. Consequently, many researchers advocate the use of "space filling" designs when sampling deterministic computer analyses to treat all regions of the design space equally. A comparison of these designs is in Ref. [53].*

Fasihul et al. [14] investigates the effect of experimental design on the development of neural network simulation metamodel. The experimental design approaches used are CCD, a modified Latin Hybercube design, and designs supplemented with domain knowledge. The neural network developed from modified Latin Hybercube design supplemented with domain knowledge produces the best performance. In another paper, Fei et al. [54] seven sampling techniques were used to evaluate the accuracy of neural network model. Two benchmark problems; an antenna model and an aircraft model was used and the result showed that the uniform design is the best sampling technique for metamodel building. Isabel et al. [55] proposes a sequential design that improves the accuracy of the nonlinear simulation metamodels. The paper also stresses that a careful choice of an experimental design can lead to better metamodels, with the same simulation effort.

Model types

The next step after the selection of experimental design is to perform the necessary computer runs and to choose an approximating model. Many model types are available of which RSM that uses polynomial functions and neural network are the well known approaches. RSM, the most well-established metamodeling technique, is a popular and an easy method for approximation. It is quite suitable and effective in engineering design applications due to its simplicity when the number of design variables is small and the response is not highly nonlinear. RSM are often in form of low order polynomials. Among these common models, the quadratic polynomial response function is the most popular. Fasihul et al. [14] investigates the effect of experimental design on the development of neural network simulation metamodel.

Many literatures have been reported work using neural networks [37,40,54,75,78,84,88,91,94,95,100]. Other types of models includes Radial Basic Functions (RBF), kriging and Multivariate Adaptive Regression Splines (MARS).Radial Basis Function (RBF) is a kind of neural network metamodeling technique that is different from RSM because RBF interpolates data and the approximate response surface goes through all the data points. It is considered that this method is excellent to fit and interpolate the response of a deterministic process of computer simulation codes. Also, when the number of design variables increases and the response is highly nonlinear, the RSM becomes less attractive because the number of design points increases correspondingly. In this case, RBF would be one of the alternative options of metamodeling techniques. Kriging (design and analysis of computer experiments), an interpolative model is becoming popular in recent years. Kriging was originally developed by the South African mining engineer called Krige and later on the model was developed by Sacks et al. [7,56]. A recent review on kriging metamodeling is available in Jack et al. [57]. Despite the several approximation methods, the comparative studies among these approaches are limited. Giunta, et al. [58] compared the polynomial and interpolating (kriging) models through test problems involving one, five and ten variables. Some researchers like Jin, et al.,[8], Simpson et al. [1, 59] and Forrester et al.[5] have compared the metamodeling methods and their progress in the past two decades.

Application to Design optimization

Wang et al. [60] uses the metamodel generated using RSM and kriging to optimize a cylindrical tube impacting a rigid wall which involves nonlinearity, buckling, and dynamics. In the same paper another problem of topologic optimization of initial blank shape was also performed. Jouhaud et al. [61] applied the metamodel based shape optimization method in case of the multidisciplinary shape optimization of a 2D NACA subsonic airfoil. Sakata et al. [62] solved a problem on layout optimization of a beam structure for eigen value maximization. Stinstra et al. [63] applied the metamodel based optimization method to the design of two parts of the TV tube: furnace profile and shadow mask. Dellino et al. [64] uses the kriging metamodel in multi-objective engineering design optimization of a injection system for compressed natural gas engines. Sakata et al. [31] investigates the applicability of kriging to minimize the thermoelastic deformation by the piezoelectric effect of a composite structure. They use an optimization method to determine the optimum applied electric potential to minimize the thermoelastic deformation. Raza et al. [22] combines the Reynolds-averaged Naveir stokes analysis with kriging method in the shape optimization of a wire-wrapped fuel assembly in a liquid metal reactor. The optimization problem in this case is stated as the maximization of the objective function, which is defined as a linear combination of heat transfer and friction related functions with a weighting factor. Two design variables are selected and design points are chosen using Latin Hypercube Sampling. Sakata et al.[65] created a metamodel for layout optimization of beam reinforcement and the response surface for the reinforcement effect of inserted additional elements was estimated. Gano et al. [66] used kriging model for the sizing problem of an internal combustion engine and for a control-augmented structural design problem. In the former case, the geometry for a flat head internal combustion chamber is sought to provide maximum specific power satisfying a number of constraints such as fuel *economy, packaging and knock limitations. The objective of the control-augmented structure design problem is to minimize the total weight of the structure. This minimization problem is subjected to certain constraints like, static stresses, lateral and rotational displacements, natural frequencies and dynamic lateral and rotational displacements. Meunier et al. [67] used kriging to model the behavior of shape memory alloy(SMA)s that are nonlinear functions of several variables, thus, permitting design optimization. Trochu et al. [68] uses dual kriging to model the hysteretic material laws of SMA. This model was interfaced with a nonlinear finite element program to analyze the SMA devices. Finally, two industrial examples: a SMA spring-disk developed for electrical contacts and a SMA medical dent was analyzed for design optimization.*

Application to reliability based design

Malur et al. [69] presented an iterative procedure to develop a response surface that is locally a good approximation to the actual limit state surface in the region of maximum joint probability density and can be used for structural reliability analysis. He also suggests that the response surface method can be used effectively for reliability analysis of certain structural systems where behavioral models to describe their various limit states cannot be developed in closed form. Das et al. [70] have proposed an improved RSM in which the function has constant, linear, and selected quadratic terms. Improvement in the performance of response surface function was made by including or removing some of the second order terms. In this way an appropriate incomplete second order response surface was obtained. Similar work has been carried by the same authors [71] and has used a stiffened plate under combined load for the reliability study. Tandjiria et al. [72] have applied RSM for the reliability analysis of laterally loaded piles. The reliability results calculated using MCS and RSM agreed well with only slight differences in the failure probability due to the assumptions made. Pendola et al. [73] presented a probabilistic methodology for nonlinear fracture analysis of general cracked structures. Two methods are studied for the coupling of finite element analysis with reliability software. An example of a cracked pipe was presented to illustrate the proposed methodology. The results also showed that the methodology was able to give accurate probabilistic characterization of the J-integral in elastic-plastic fracture mechanics without obvious time consumption. Guan et al. [74] highlights the possible effects on the response surface model due to the variation in the experimental design points. Hurtado et al. [75] summarized the applicability of different kinds of neural networks for the probabilistic analysis of structures. The comparison was made between multi-layer preceptors and radial basis functions classifiers and over four examples. The paper also indicates some recommended ways of employing neural networks. Soares et al. [76] described a formulation to compute the reliability of reinforced concrete structures, in which physical and geometrical non-linearities are taken into account. The non-linear model adopted allows the representation of the mechanical behavior of concrete structures at the failure stage, which is governed by possible large displacement effects, softening behavior of concrete and tension stiffening effects. The failure surface is obtained by fitting the internal force ultimate state of the structure using a quadratic polynomial. Assessing the reliability of a complex structure requires a deal between reliability algorithms and numerical methods used to model the mechanical behavior. The RSM represents a convenient way to achieve this purpose. The interest of such a method is that the user is allowed to choose and check the computed mechanical experiments. Nevertheless, this choice in an optimal way turns out to be not always an easy task. Gayton et al. [77] proposed a response surface method named CQ2RS (Complete Quadratic Response Surface with Re-Sampling) allowing to take into account the knowledge of the engineer on one hand and to reduce the cost of the reliability analysis using a statistical formulation of the RSM problem on the other hand. Some academic and industrial examples were presented to illustrate the efficiency of the method. The MCS, the First-Order Reliability Method (FORM) and the Second-Order Reliability Method (SORM) are the three common reliability analysis methods used for structural safety evaluation. The MCS requires calculations of several performance functions while FORM and SORM demands partial derivatives of the performance function with respect to the design variables. Such calculations are time consuming. In order to address these issues, Deng et al. [84] presented three Artificial Neural Network(ANN) based reliability analysis methods, i.e. ANN-based MCS, ANN-based First Order Reliability Method and ANN-based Second Order Reliability Method. Examples were given in this work to illustrate the procedure of this method. Gomes et al. [78] in their work presented the RSM and ANN techniques and compared these techniques using FORM, Direct MCS and MCS with adaptive importance sampling technique. Problems with simple limit state functions and closed form solutions of the failure probability are solved in order to highlight the advantages and disadvantages using these techniques. It is observed that in problems where the computational cost of structural evaluations is high, these two techniques may turn feasible the evaluation of the structural reliability through simulation techniques. The problem of response surface modeling of limit surface within two hyper spheres of prescribed radii is considered in Gupta et al. [79]. The relevance of this problem in structural reliability analysis involving performance functions with multiple design points that make significant contributions to failure probability is discussed. The paper also proposes global measures of sensitivity of failure probability with respect to the basic random variables. The performance of the proposed improvements is examined by comparing the simulation based results with results from the proposed procedure with reference to two specific structural reliability *analysis problems. A probabilistic design system for reliability based design optimization problems called ADAPRES_NET was presented by Kaymaz et al. [80]. ADAPRES_NET includes two main features, one of which is the use of an adaptive response surface method by which the response functions, the other distributed computing environment by which the computational applications are distributed on a network. The proposed system was presented with a connecting rod example and evaluation of the probabilistic constraints was also compared with that of the classical reliability methods, and the results indicated the benefits of using this technique. Qu et al. [81] proposed a probabilistic sufficiency factor approach that combines safety factor and probability of failure. The approach provides a measure of safety that can be used more readily than the probability of failure to estimate the safety level. The paper presents the use of probabilistic sufficiency factor with a design response surface approximation, which fits it as a function of design variables. It is also shown that the design response surface approximation for the probabilistic sufficiency factor is more accurate than that for the probability of failure or for the safety index. Rais-Rohani et al. [82] discussed the development and application of global and local response surface techniques for the solution of reliability based optimization problems. A thin walled composite circular cylinder under axial buckling instability was used as a demonstrative example. The two techniques adopted are found to produce similar results in terms of accuracy, with the sequential local RS technique having a considerably better computational efficiency. Youn et al. [83] integrated the hybrid mean method with response surface method for reliability based design optimization of vehicle side impact problem. The design objective is to enhance side impact crash performance while minimizing the vehicle weight. Kaymax [85] investigates the use of the kriging method for structural reliability problems by comparing it with the most common RSM. The effects of the kriging parameters are also examined on the basis of the reliability index computation and fitting behavior. Some advantages and disadvantages of the kriging model are reported based on the results obtained from the application of the kriging method to the examples from literature. In continuation of his earlier work Kaymaz et al. [85, 86] uses a weighted regression method in place of normal regression in his proposed ADAPRES system. Examples are given in this paper to demonstrate the benefit of the proposed method for both numerical and implicit performance functions. Leira et al. [87] has investigated the application of response surface for reliability analysis of marine structures subjected to multiple environmental loads. The structural fatigue damage and long term response are expressed in terms of these environmental parameters based on application of polynomial response surfaces. Schueremans et al. [88] propose a technique to increase the efficiency of simulation based reliability algorithms. The low order polynomial response surfaces are extended using neural networks and splines. The reliability framework was presented, compared with traditional RSM and commented extensively. The overall behavior of the technique was addressed referring to several benchmark examples. Wong et al. [89] presented a case study to investigate the cause for the divergence of the solution of the reliability analysis. An adaptive design approach was proposed to overcome this problem and several suggestions are made to improve the robustness of the RSM. Three numerical examples have been chosen to demonstrate the proposed method, which was verified by MCS. Deng [90] proposed three RBF network methods to compute the implicit performance function and then to combine them with conventional MCS, FORM and SORM and propose three RBF reliability analysis methods: RBF based MCS, RBF based FORM and RBF based SORM. The presented methodology is convenient for problems with highly non-linear performance functions or with large number of random variables. The author in his first paper, Deng et al. [84], used NN instead of RBF. Similar work has been carried out by Elhewy et al. [91] and paper shows that the ANN-based RSM is more efficient and accurate than the conventional RSM. In Babu et al. [92] the concept of RSM was used to generate the approximate polynomial functions for ultimate bearing capacity and settlement of a shallow foundation resting on a cohesive frictional soil for a range of expected variation of input soil parameters. Considering the variations in the input soil parameters, reliability analysis is performed using these response surface models to obtain an acceptable value of the allowable bearing pressure. Bucher et al. [93] presented an overview of approximation techniques like RSM, moving least square regression, RBF and NN and demonstrates their potential in structural reliability analysis. Cheng et al. [94] developed a new class of ANN based Genetic Algorithm (GA) for reliability analysis of structures. The method involves the selection of training datasets by uniform design method, approximation of the limit state function by ANN and estimation of failure probability using the GA. Three example problems illustrated the benefits of integrating uniform design method, ANN and GA and indicated that the proposed method provide accurate and computational efficient estimates of probability of failure. Similar work has been carried out by Cheng et al. [95] in which FORM is used for estimating failure probability. Hao et al. [96] has studied the reliability based optimization of composite structures by combining RSM and finite element method. Jansson et al. [97] evaluated the use of linear and quadratic approximating response surfaces as metamodels in the reliability assessment of a sheet metal forming process using the MCS technique. The studies showed that linear metamodels can be used to identify the important variables and to give an estimate of the probabilistic response. And quadratic surfaces are required for more accurate analysis. Lee et al. [98] proposed constraint boundary sampling to build metamodel that can predict optimum point accurately while* *satisfy constraints. This technique is applied to the design of double-deck car body and was compared with conventional space-filling sampling. Fong et al. [99] developed a response surface as a surrogate for the thermal-hydraulic code for the selection of an ultimate heat sink for a passive secondary auxiliary cooling system. The reliability of the chosen design during the bounding transient, a station blackout was calculated. The uncertainty introduced by the use of the response surface itself was explored. Moller et al. [100] addressed an approach to performance based design in the context of earthquake engineering. The objective is the optimization of the total structural cost, under constraints related to minimum target reliabilities specified for the different limit states or performance requirements. The approach uses a neural network representation of the responses. Moller et al. [101] presented a comparison between three methods for the implementation of response surfaces: a global approximation of the deterministic database, local interpolation of that database, or using artificial neural networks. The comparison uses, an example, a 5 storey reinforced concrete building. The results showed good agreement between the methods and the paper discussed their corresponding advantages and limitations.*

RECOMMENDATIONS, GUIDELINES AND CHALLENGES

In this paper, we have discussed the concept of metamodeling and survey the advancements in the metamodel based analysis within design optimization and reliability based design application in the past thirty years. Most metamodeling applications are based on low order polynomials using CCD and least square regression (RSM technique). The main limitation of the RSM is the use of single low order polynomial to represent the function. Many systems cannot be described well using a single low order polynomial. In order to accurately define the real system, use of more piecewise low order polynomials or Splines can be made. These piecewise continuous polynomials allow more complex system behavior to be redefined in small areas. Neural Networks (NN) is also another perspective to the above criteria. The weighting function which is the basis of the network, are very flexible and can adapt to any kind system behavior. Therefore, NN has no limits on shape, dimension and type of function. Kriging, an interpolation method capable of handling deterministic data which is extremely flexible due to the wide range of correlation functions may be chosen. However, the method is more complex than RSM. The opinion on the appropriate experimental design for computer analyses vary; the only consensus reached thus far is that design for non-random, deterministic computer experiments should be space filling designs [3].

Though intensive research on metamodeling has been carried out some research challenges remain to be overcome. It was recognized that when the number of design variables is large, the total computation expense for metamodel based analysis makes the approaches less attractive or even infeasible. For eg, if CCD and a second order polynomial function are used for metamodeling, the minimum number of sample points required is $2^n + 2n + 1$*, where n is the number of design variables. There seems to be a lack of research on large-scale problems. New metamodeling techniques for large-scale problems, or simple yet robust strategies to decompose a large scale problem, are needed. In summary, the following conclusions can be made:*

- *Space filling designs are the best experimental design than classical designs*
- *If the problem involves more number of design variables, neural networks and radial basis functions may be the best choice despite computationally expensive to create*
- *If the problem to be modeled is highly nonlinear and with the number of design variables less than 50, then kriging may be the best*
- *Application with few variables and the behavior is smooth with less nonlinearity, and then response surface methodology may be used.*

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