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Design and Analysis of Computer Experiments in Multidisciplinary Design Optimization: A Review of How Far We Have Come – or Not

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The use of metamodeling techniques in the design and analysis of computer experiments has progressed remarkably in the past two decades, but how far have we really come? This is the question that we investigate in this paper, namely, the extent to which the use of metamodeling techniques in multidisciplinary design optimization have evolved in the two decades since the seminal paper on Design and Analysis of Computer Experiments by Sacks et al. As part of this review, we examine the motivation for advancements in metamodeling techniques from both a historical perspective and the research itself. Based on current thrusts in the field, we emphasize multi-level/multi-fidelity approximations and ensembles of metamodels, as well as the availability of metamodels within commercial software and for design space exploration and visualization in this review. Our closing remarks offer insight into future research directions – nearly the same ones that have motivated us in the past.

I. Introduction

DESIGN and analysis of computer experiments, or DACE as it has become known, was introduced twenty years ago by Sacks et al.[1] to refer to the set of methodologies for generating metamodels for computer codes used for analyses during multidisciplinary design optimization (MDO). We consider metamodeling to be the general process of creating an abstraction (approximation or interpolation) of an underlying phenomena (i.e., a response) over a certain domain – creating a "model of the model" as defined by Kleijnen.[2] In the general scope of metamodeling, a response may be evaluated via a physical experiment or a computer simulation at a number of points in the domain. Our review will further focus on work dealing primarily with DACE, which is different from traditional Design of Experiments – developed primarily for performing physical experiments[3] – in that data generated from computer experiments is deterministic in nature, i.e., for the same set of inputs, one gets the same set of outputs. In our review we consider metamodels that can either interpolate the values of the response at certain points or provide a "best fit" based on some metric (e.g., sum of squares of errors at a number of points). Common types of metamodels include spline, polynomial (e.g., response surface), kriging, radial basis functions, neural networks, etc. The common feature of all these approaches is that the actual response is known at a finite number of points, but the metamodel is created for a certain domain and is then used as a surrogate for the original model, i.e., it provides a substitute for and is used in lieu of the original computer model. In this work, surrogate model is synonymous with metamodel.

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Our goal in this review is to investigate how far metamodeling techniques have come – or not – since the introduction of DACE nearly two decades ago. Our goal is not to provide a comprehensive review given the extensive literature reviews that have appeared recently.[4,5] Instead, we first take a historical perspective in Section II to explore how the research, and more importantly how the motivation for the research, has evolved this past twenty years. We then discuss four research areas that have benefited from metamodeling while also driving research in the area: (1) multi-level and multi-fidelity approximations (Section III), (2) the use of multiple surrogates and metamodel ensembles (Section IV), (3) metamodeling capabilities in commercial software packages (Section V), and (4) metamodel-based design space exploration and visualization (Section VI). Section VII provides our closing remarks and highlights future work – much the same as what has been motivating us for the past two decades.

II. History of Development

A. Origins and Early Uses

Approximation methods in MDO have their origins in structural synthesis[6,7] and have been applied to a wide variety of structural design problems.[8] Approximation methods are often classified as being either global or local:[8] *global* approximations are valid throughout the entire design space (or a large portion of it) while *local* approximations are only valid in the vicinity of a particular point. Mid-range approximations also exist for creating local approximations with global qualities.[9] Approximations are also used to facilitate the integration of discipline-specific computer analyses and can provide better insight into the relationships between design (input) variables and system performance (output) responses. An added benefit of some approximation methods is smoothing numerically "noisy" data, which can hinder the convergence of many optimization algorithms.[10,11,12]

Prior to 1990, polynomial response surface models, first introduced by Box and Wilson[13] and later detailed in Ref. 14, and neural networks[15] were among the most popular approximation methods. Early contributors to approximation method development for MDO include research groups at the Virginia Institute of Technology, the University of Notre Dame, Rensselaer Polytechnic Institute, Old Dominion University, and the NASA Langley Research Center. A review of applications of response surface models, neural networks, and other types of approximations in MDO during this time can be found in Refs. 8,16.

B. Developments in the 1980's and 1990's

The prohibitive computational cost of the direct combination of FEM with methods of mathematical programming stimulated the idea of approximation concepts based on the information from the first order design sensitivity analysis.[7] Since then this concept of sequential approximation of the initial optimization problem by explicit sub-problems has proven to be very efficient. As examples the methods can be named such as the Sequential Linear Programming (SLP) used for structural optimization problems by Pedersen,[17] the CONvex LINearization method (CONLIN) by Fleury and Braibant,[18] and Fleury,[19,20] the Method of Moving Asymptotes (MMA) by Svanberg.[21] All of these methods use the information obtained from response analysis and first-order design sensitivity analysis (i.e., values of functions and their derivatives) at a current point of the design variable space and hence can be classified as single point approximation methods. Note that all the information from previous design points is discarded. Later on, several first-order approximation techniques have been developed based upon the function value and its derivatives at the current and the previous design points (two-point approximations): Haftka et al.,[22] Fadel et al.[23] The main purpose is to improve the quality of approximations and thus reduce the number of iterations needed to solve the optimization problem and the total optimization time. Rasmussen[24] developed this idea further, his Accumulated Approximation technique (ACAP) used function values and derivatives at a current design point and the function values obtained at all previous points. Toropov[25] introduced a technique that used function values gained in each iteration at several previous design points (multipoint approximations). The aim was to combine the benefits of the two basic approaches, hence the technique can be classified as a mid-range approximation. Later this technique was expanded to incorporate the design sensitivities (when available) into the approximation building.[26]

A different approach to structural optimization[27] is to create approximate explicit expressions by analysing a chosen set of design points and using response surface methodology. This approach is based on the multiple regression analysis which can use information being more or less inaccurate. They are global in nature and allow designers to construct explicit approximations valid in the entire design space; however, they are restricted by relatively small optimization problems (up to ten design variables[27]). This approach was used for solving various structural optimization problems by Schoofs,[28] Vanderplaats,[27] Rikards.[29]

Interest in approximation methods and metamodeling techniques grew substantially in the 1990s, particularly within the MDO community. During the first half of the decade, heavy emphasis was placed on response surface methods, which primarily resulted from NASA-funded research related to the High Speed Civil Transport (HSCT). Researchers at the Virginia Institute of Technology, University of Notre Dame, Georgia Institute of Technology, Rice University, and Old Dominion University continued to advance the state-of-the-art by developing novel methods and uses for response surface models. Many of these efforts were chronicled at the *1995 MDO Workshop* sponsored by ICASE/NASA Langely.[30,31,32,33,34] For instance, the Variable Complexity Response Surface Modeling (VCRSM) method developed predominantly at Virginia Tech,[35,36] uses analyses of varying fidelity to reduce the design space to the region of interest and build response surface models of increasing accuracy. The Concurrent SubSpace Optimization procedure from Notre Dame uses data generated during concurrent subspace optimization to develop response surface approximations of the design space which form the basis of the subspace coordination procedure during MDO.[37,38,39] Robust Design Simulation[40] and the Robust Concept Exploration Method[41,42] were developed at Georgia Tech to facilitate quick evaluation of different design alternatives and generate robust top-level design specifications. Hafkta et al.[43] and Simpsonet al.[44] provide extensive reviews of response surface and approximation methods in mechanical and aerospace engineering during this timeframe.

As response surface modeling became more widely used and better understood, its limitations became more apparent, e.g., the "curse of dimensionality"[45,46] and the inability to create accurate global approximations in highly non-linear design spaces.[47] As a result, some researchers started exploring higher order response surface models[48] and mixed polynomial models[49] while others investigated more efficient experimental designs for sampling the design space using computer analyses.[50,51,52] Other researchers also started investigating the use of gradient information to facilitate metamodel construction.[53,54,55] Sequential approaches to sampling, building, and optimizing approximation models were also being investigated by many researchers, and the use of move limits[12] and trust region approaches[56,57] were being advocated by many researchers for sequential metamodeling. This led to the development of mathematically rigorous techniques to manage the use of approximation models in optimization such as the Surrogate Management Framework,[58] developed collaboratively by researchers at Boeing, IBM, and Rice University. During this time frame, many companies also started to develop software to facilitate the use of approximation methods in design and optimization: iSIGHT[59] by Engineous Software, Inc.; Visual DOC[60] by Vanderplaats R&D, Inc.; Optimus[61] by LMS International; ModelCenter[62] by Phoenix Integration; Design Explorer[58] by The Boeing Company; and DAKOTA[63] by Sandia National Laboratories. Section VI gives a more detailed review of the metamodeling capabilities within each of these software packages.

C. 2000 to Today

In the latter part of the 1990s, the emphasis also started to shift away from response surface models to alternative approximation methods such as radial basis functions,[64,65,66] Multivariate Adaptive Regression Splines,[67] Kriging,[1,68] which was the focus in many dissertations,[69,70,71,72] and more recently, support vector regression.[73,74] The availability of alternative methods led to many comparative studies to determine the advantages of different metamodeling techniques.[75,76,77] The merits of various metamodeling techniques were discussed extensively at the *Approximation Methods Panel* held at the *9th AIAA/ISSMO Symposium on Multidisciplinary Analysis & Optimization.*[5] As discussed in the panel, metamodels are finding a variety of new uses, including optimization under uncertainty, which is receiving considerable attention as of late,[78] and robust design and reliability-based design since they provided inexpensive surrogates for Monte Carlo simulation and uncertainty analysis.[79]

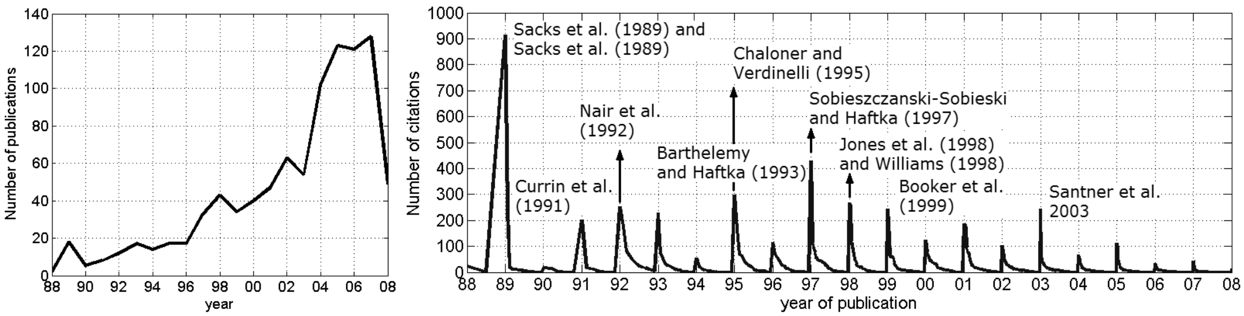
This evolution is summarized well in Figure 1, which shows the number of DACE-related publications over the past twenty years. This data was obtained using the Publish or Perish software system[**] and Google Scholar[††] where we searched for occurrences of the phrase: "design and analysis of computer experiment." While the specific results may vary slightly as the Google database is updated, we see a steady growth in the number of papers on DACE, especially in the last decade (see Figure 1a). In Figure 1b, publications are sorted according to the number of citations to complement the information in Figure 1a. In each year, at least one paper is likely to receive more than 100 citations; in fact, 24 papers have more than 100 citations and 11 more than 200 citations. It is clear that the focus on DACE rewards authors with citations.

Figure 2 (adapted from Viana and Haftka[80]) illustrates the number of publications reporting the use of some of the major surrogate techniques. Data was also obtained using the Publish or Perish software system and Google Scholar (in the period of June 10-25, 2008). For each technique, Viana and Haftka[80] searched for occurrences with any of the following words: interpolation, approximation, metamodel, regression, classification, prediction. In practice, for example for "response surface", the search in Google Scholar is fed with: interpolation OR approximation OR metamodel OR regression OR classification OR prediction AND "response surface". These

[**] http://www.harzing.com/pop.htm accessed on June 24, 2008
[††] http://scholar.google.com accessed on June 24, 2008

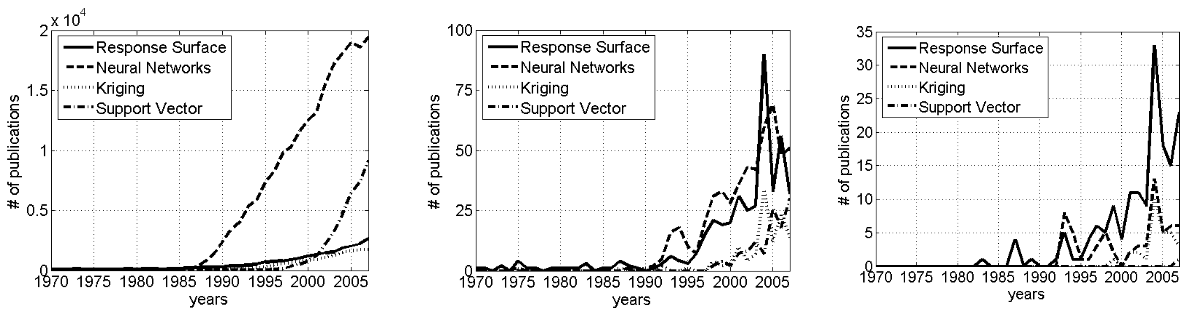
results may also vary due to the update on the Google database. Figure 2a shows an impressive growing of publications on neural networks when there is no restriction on the research field (the same for support vector since the beginning of this decade). Figure 2b illustrates what happens in the optimization community, where the 1990's trigged the popularity of surrogate techniques. Figure 2c narrows even further the numbers to the scope of the structural optimization community; where response surface still seems to be the favorite technique. The lessons that we can take from these pictures are:

- In terms of the large spectrum of regression applications: different surrogates are equally competitive.[80]
- In terms of history: the popularity of DACE is interconnected to the developments on individual surrogate techniques.



(a) Number of publications, from 1988 to 2008 (b) Number of citations by year of publication, from 1988 to 2008.

Figure 1. Statistics for publications containing the phrase "Design and Analysis of Computer Experiments."



(a) Metamodels in all areas (b) Metamodels in optimization (c) Metamodels in structural opt.

Figure 2. Number of publications by year for four types of metamodels (adapted from Viana and Haftka[80]).

To identify the motivation for metamodeling research, consider Table 1, which summarizes frequently-cited review papers published in the past two decades. One thing that is immediately evident is the common theme in all of these papers is the high cost of computer simulations, e.g., "despite growing in computing power, surrogate models are still cheaper alternatives to actual simulation models in engineering design." This statement is still weak in the sense that one could argue that with the computational resources that we have today, instead of using surrogate models for approximation purposes, we could rely on low-fidelity codes (or alternatively, codes that used to be high-fidelity models in the past but that would run much faster in today's computers). The devil's advocate would say that both surrogate and the cheap low-fidelity models would bring a level of uncertainty (compared with the current high-fidelity simulations); however, the latter would have the advantage of being already well-know and used (besides, it would save one to go to the sampling issues on surrogate modeling).

To be fair, let us start by asking: what have the advances in computational throughput been used for in different segments of the engineering design? Figure 3 helps us to see that if it is true that the advances have helped the development of numerical optimization; they also seem to favor an increase in complexity of the state-of-the-art simulation.[81] In general, we can see that the computational resources were used to add complexity; so, it is likely that one could not use old high-fidelity models to obtain the output of some of the today's codes (take the example of the transient analysis). On the other hand, we can say that the cost of fitting a given surrogate compared to the cost of simulations has reduced over time, which helped to make more sophisticated surrogates to become popular. On top of that, surrogates such as kriging models and even the traditional polynomial response surface also offer information about the prediction error (obviously not found in old high-fidelity codes). More than just an estimator of the point-wise error in prediction, these structures can be used for rational allocation of the computational resources in the optimization process itself. For example, they can guide refinement of the design space toward regions of high uncertainty or regions where the optimization is mostly likely to improve the objective function. This is the case of algorithms such as the Efficient Global Optimization (EGO).[82] The bottom line is that the repertoire of design tools has substantially grown over the years and DACE methods helps tailoring problem-oriented approaches during the design process. The next section reviews advancements in mutli-level and multi-fidelity approximations, a topic in metamodeling that is still receiving considerable attention.

Table 1. Motivation for previous review papers about "Design and Analysis of Computer Experiments."

Paper	Year	Statement
Sacks et al.[1]	1989	Abstract: "*Many scientific phenomena are now investigated by complex computer models or codes… Often, the codes are computationally expensive to run, and common objective of an experiment is to fit a cheaper predictor of the output to the data*"
Barthelemy and Haftka[8]	1993	Introduction: "*… applications of nonlinear programming methods to large structural design problems could prove cost effective, provided that suitable approximation concepts were introduced*"
Sobieszczanski-Sobieski and Haftka[16]	1997	Abstract: "*The primary challenges in MDO are computational expense and organizational complexity.*"
Simpson et al.[44]	2001	Abstract: "*The use of statistical techniques to build approximations of expensive computer analysis codes pervades much of today's engineering design.*"
Simpson et al.[5]	2004	Introduction: "*Computer-based simulation and analysis is used extensively in engineering for a variety of tasks. Despite the steady and continuing growth of computing power and speed, the computational cost of complex high-fidelity engineering analyses and simulations maintains pace... Consequently, approximation methods such as design of experiments combined with response surface models are commonly used in engineering design to minimize the computational expense of running such analyses and simulations.*"
Wang and Shan[4]	2007	Abstract: "*Computation-intensive design problems are becoming increasingly common in manufacturing industries. The computation burden is often caused by expensive analysis and simulation processes in order to reach a comparable level of accuracy as physical testing data. To address such a challenge, approximation or meta-modeling techniques are often used.*"

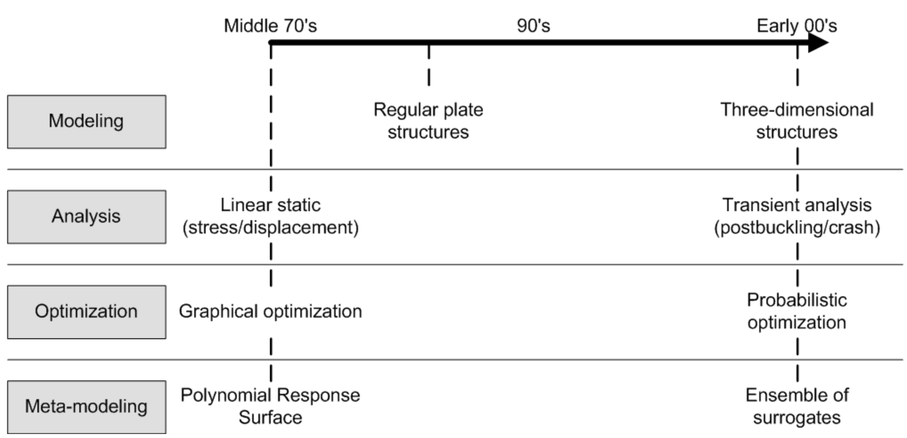


Figure 3. Bi-level summary of the evolution in the use of computational resources.[81]

III. Multi-level and Multi-fidelity Approximations

In the past two decades, we have observed a sharp increase in the number of papers on metamodeling approaches based on the interaction of high- and low fidelity numerical models. In such approaches there is an assumption that, apart from the high fidelity numerical model that is sufficiently accurate but requires a large computing effort for an evaluation, there is another one that is not as accurate but is considerably less computationally demanding. Such a model can be obtained by simplifying the analysis model (e.g., by using a coarser finite element mesh discretization, a reduced number of the natural modes of the model in dynamic analysis, etc.) or a modeling concept (e.g., simpler geometry, boundary conditions, two-dimensional instead of a three-dimensional model, etc.). A low fidelity model can provide a basis for a high quality metamodel building resulting in solving an optimization problem to the accuracy of the high fidelity model at a considerably reduced computational cost. In the metamodel building, a low-fidelity model is corrected (or tuned) using the model response values from a relatively small number of calls for both high fidelity and low fidelity models according to a suitable design of experiments. Such tuning can be refined in an adaptive way as optimization progresses. The overall objective of this approach is to attempt to circumvent the curse of dimensionality associated with black-box metamodeling by exploiting domain-specific knowledge.[83]

In some cases there can be a hierarchy of numerical models, e.g., based on Navier-Stokes equations (highest fidelity and most expensive), on Euler equations (lower fidelity and less expensive), linear panel method (lover fidelity and cheaper), etc. down to analytical or empirical formulae (e.g., obtained from the wind tunnel test data). These can be exploited to in an optimization strategy with hierarchic metamodel building and refinement.

Originally, the idea of improving quality of approximation by endowing the metamodel with some discipline-related properties of the numerical model response function stems from the empirical model-building theory. Box and Draper[84] showed that a mechanistic model, i.e., the one that is built upon some knowledge about the system under investigation, can provide better approximations than general ones, e.g., polynomials. An example of application of such a model to a problem of material parameter identification (formulated as an optimization problem) was given by Toropov and van der Giessen[85] where the structure of the metamodels of response quantities (torque and elongation) for a solid bar specimen in torsion, obtained by a nonlinear FE simulation, was derived from a simpler functional dependence on material parameters for a tubular specimen. The simplified (thin-walled tubular) model analyzed by solving an ODE, was the basis for the metamodel describing the behavior of a solid model that was analyzed by much more complex numerical simulation. The radii of the artificial tube specimen were treated as metamodel parameters used to match the two models at sampling points.

A different route to introducing approximations based on the interaction of high and low fidelity models was taken by Haftka[86] while aiming at extending the range of applicability of a local derivative-based approximation of the high fidelity response $F(\boldsymbol{x})$ at a current design point. A global approximation is also introduced that is considered to be a simple-model approximation (i.e., a low fidelity model) $f(\boldsymbol{x})$. A scaling factor $C(x_0) = F(x_0)/ f(x_0)$ can be calculated at a current design point $\boldsymbol{x}_0$ and its approximation built using Taylor series expansion. This allows creation of an extended range approximation to the high fidelity response by correcting (scaling) the low fidelity response $\tilde{F}(\boldsymbol{x}) = f(\boldsymbol{x})\, C(\boldsymbol{x})$ ensuring that the values and the derivatives of the high fidelity response coincide with those of the scaled low fidelity response. This approach was termed Global-Local Approximation` (GLA) method and demonstrated on a beam example with a crude and more refined FE models. Later, this approach was termed Variable Complexity Modeling (VCM) technique and used by Unger et al.[87] alternating calls for the low and high fidelity models to update the correction applied to the low fidelity model during the optimization. The same approach was applied to optimization problems with response functions related to aircraft structural performance[88] and aerodynamics.[89]

A rigorous implementation of an approximation management framework (AMF) based on the scaling of the low fidelity response and incorporating a trust region strategy is presented in Alexandrov et al.[90] The term approximation is used to define any model that is less expensive than a high fidelity model, including low fidelity numerical models, response surfaces, kriging metamodels, etc. Several examples are given including optimization of a 3D wing parameterized with 15 design variables where both high and low fidelity (8 times less expensive) models were based on Euler simulation (incorporating an automatic differentiation tool) of different grid refinement achieving a threefold saving in computing effort. An application of this framework, renamed approximation and model management framework (AMMF), to optimization of two-element airfoil utilizing a Reynolds-averaged Navier-Stokes (RANS) code and an Euler code as high- and low fidelity simulation tools, respectively,[91] resulted in the run time ratio of 55:1 (excluding sensitivity analysis performed by an adjoint approach) and achieved a fivefold saving in computing effort. Second order correction methods that require second derivatives of the high- and low fidelity response were introduced by Eldred et al.[92] implemented in the DAKOTA software[63] and compared to other metamodeling techniques.[93]

Knill et al.[94] stated that the gradient-based low fidelity model correction procedure was effective in reducing the computational cost but it was adversely affected by the presence of numerical noise in aerodynamic and structural response values. To circumvent this, Giunta et al.[95] suggested to initially perform a thorough design space exploration utilizing a low fidelity model, and identify and exclude “non-sense” regions arriving at a much reduced ribbon-like domain in the design space. This allowed building a polynomial response surface of the high fidelity response utilizing a much reduced number of sampling points in the aerodynamic design of a High Speed Civil Transport (HSCT) aircraft wing. This number could be further reduced by performing an ANOVA study on a low fidelity response surface in order to identify less significant terms in a polynomial regression model and remove them from the polynomial response surface for the high fidelity response.[32] Another benefit of performing a preliminary response surface building on a low fidelity model is that it allowed to identify a set of intervening functions that are easier to approximate by a polynomial response surface separately and use those to construct a response or the original complex function, such as wing bending material weight of a HSTC.[96] Later, this approach was further enhanced by establishing a polynomial response surface for the correction function from a relatively small number of calls for te high fidelity model (as compared to the sampling size used to run the low fidelity model), that is then utilized to correct the low fidelity model by applying correction to its polynomial approximation[97] or to the data used for its creation. Balabanov et al.[98] compared these two approaches and found the difference in the quality of the obtained approximation rather small. Venkataraman and Haftka[99] demonstrated the effectiveness of correcting inexpensive analysis based on low fidelity models by results from more expensive and accurate models in the design of shell structures for buckling. Vitali et al.[100] used a coarse low fidelity finite element model to predict the stress intensity factor, and corrected it with high fidelity model results based on a detailed finite element model for optimizing a blade-stiffened composite panel. In the optimization of flow in a diffuser, parameterized with 6 design variables, Madsen and Langthjem[101] used Navier-Stokes CFD solution with a fine grid as a high fidelity model and experimented with two models of lower fidelity, an empirical formula and a coarsened CFD grid arriving at an acceptable solution with 14 calls for the high fidelity model.

Toropov and Markine[9] generalized the metamodeling approach based on the interaction of high and low fidelity models by considering a metamodel as a tuned low fidelity model:

$$\tilde{F}(\mathbf{x}, \mathbf{a}) \equiv \tilde{F}(f(\mathbf{x}), \mathbf{a}) \approx F(\mathbf{x}) \quad , \tag{1}$$

where $f(\boldsymbol{x})$ is the low fidelity response and $\boldsymbol{a}$ is a vector of tuning parameters used for minimizing the discrepancy between the high fidelity and the low fidelity responses at sampling points. They suggested three types of low-fidelity model tuning:

- Type 1: Linear and multiplicative metamodels with two tuning parameters
- Type 2: Correction functions
- Type 3: Use of low fidelity model inputs as tuning parameters

The linear and multiplicative functions of Type 1 and Type 2 correction functions have been successfully used for a variety of design optimization problems.[102] The Type 3 metamodel, similarly to mechanistic models, is based on deeper understanding of a process being modeled, which can be useful but is problem-dependent. Toropov et al.[103] gave an illustrative example of a four-link mechanism optimization where the cross-sectional areas of the three movable links are chosen as the design variables. The optimization problem is to minimize the total mass of the system subject to constraints on the maximum values of the bending stresses in the links over a fixed period of time. The bending stresses are evaluated using the values of the bending moment $\sigma_i(\boldsymbol{x},t) = \left(4\sqrt{\pi}/x_i^{3/2}\right)M_i$ where M_i is the bending moment evaluated in the i-th link of circular cross-section. The following explicit mechanistic approximations of the constraint functions have been suggested: $\tilde{F}_1(\boldsymbol{x}) = a_1\,(4x_2 + x_3)\,x_1^{-3/2}$, $\tilde{F}_2(\boldsymbol{x}) = a_2 x_2^{-1/2}$, $\tilde{F}_3(\boldsymbol{x}) = a_3 x_3^{-1/2}$. The dynamic analysis of a flexible mechanism (high fidelity model) is a time-consuming procedure as it requires integration of a system of nonlinear differential equations of motion. A model with rigid links for which the dynamic analysis is two orders of magnitude faster was then used as a lower fidelity model. Since the stress distribution along the link depends on its inertia properties, the mass densities of the links have been chosen as the tuning parameters to construct the approximations of the third type (5), namely $a_i = \rho_i$, $i = 1, 2, 3$. The results of optimization indicated that the quality of mechanistic approximations was the best. followed by (from best to worst) Type 2 in multiplicative form (4) with multiplicative correction function; Type 3 (5); Type 2 in linear form (3) with linear correction function; Type 1 in multiplicative form (2). The quality of the metamodel of Type 1 in linear form (1) was unacceptably low.

Zadeh and Toropov[104] implemented the multi-fidelity metamodeling approach within the Collaborative Optimization MDO framework defining the metamodels in the whole range of design variables. Hino et al.[105] applied it to a metal forming problem where the coarser (seven times faster) low fidelity FE model was utilised resulting in the reduction of the total run time by the factor of 6.7 as compared to the use in optimization of the high fidelity FE model only. The initial sampling was done according to a small scale optimum Latin hypercube DOE (five points in the four design variable space), the low fidelity metamodel tuned and used in optimization. At the obtained point the high fidelity model was called and the responses were compared to the ones from the metamodel. A constraint violation was deemed unacceptable hence the new point was added to the DOE and the low fidelity model tuned again. In the weighted least squares metamodel tuning (6) the weights depended on the values of the objective function and constraint functions resulting in the allocation of higher weights to the sampling points located closer to the boundary of the feasible region and (from the second iteration) closer to the newly added point. After the second optimization run the obtained design was evaluated again by the high fidelity model producing only a small difference from that from the metamodel, this was taken as the solution.

An alternative approach[9] is to use the tuned low fidelity model as a mid-range metamodel within a trust region framework of the Multipoint Approximation Method.[25,26] This was applied to multibody optimization problems[103,106] and design of the embedded rail structure with a 3D FE high fidelity model and 2D FE low fidelity model.[107] Goldfeld et al.[108] considered optimization of laminated conical shells for buckling where the high fidelity analysis model (based on accurately predicted material properties) was combined with the low fidelity model (based on nominal material properties) by a correction response surfaces that approximate the discrepancy between buckling loads determined from different fidelity models.

Rodriguez et al.[109] showed that metamodels constructed from variable fidelity data generated in the concurrent subspace optimization (CSSO) MDO strategy can be effectively managed by the trust region model management strategy and gave a proof of convergence for the metamodel based optimization algorithm that has been applied to MDO test problems. Rodriguez et al.[110] extended this work to present a comparative study of different response sampling strategies within the disciplines to generate the metamodel building data.

Several researchers applied advanced metamodeling concepts to build a high quality approximation for a correction factor. Keane[111] described an aircraft wing optimization system based on the use of kriging response surface of the differences between the two drag prediction tools of different levels of fidelity. Gano et al.[112] built kriging-based scaling functions combined with a trust region-managed scheme and proved it to converge to the solution of the higher fidelity model. Gano et al.[113] enhanced this approach by introducing a metamodel update management scheme based on the trust region ratio to reduce the cost of rebuilding kriging models by updating the kriging model parameters only when they produce a poor approximation. It was found that the kriging model parameters can be updated by local methods thus improving the overall performance of the algorithm.

Leary et al.[114] developed a knowledge-based kriging model that is exhibits a performance similar to the knowledge-based ANN approach, but is preferred as being simpler to train. Forrester at al.[115] combined co-kriging (extension of kriging for the case of several responses) with a Bayesian model update criterion based on an error estimate that reflects the amount of noise in the observed data, and demonstrated the approach by a wing aerodynamic design problem. Balabanov and Venter[116] used gradient-based optimization where the one-dimensional search points are evaluated using high-fidelity analysis and the gradients are evaluated using low-fidelity analysis resulting in a multi-modeling optimization scheme that does not require correlation between the results of the high- and low-fidelity analyses.

An alternative approach termed Space Mapping also utilizes high- and low fidelity models but aims to establish a mapping of one model's parameter space on the other model's space such that the low fidelity model with the mapped parameters accurately reflects the behavior of the high fidelity model. Both linear and non-linear mappings have been considered in the literature (see, e.g., Bandler et al.,[117] Bakr et al.,[118] and Koziel et al.[119] for details) and a trust region methodology was incorporated.[120] The main difference between the previously discussed approaches where the results of the low fidelity models are in some way tuned to match those of the high fidelity model, and the space mapping approach is that in the latter a design variable space distortion is applied to the design variables of the low fidelity model to cause its optimum point to match that of the high fidelity model. A simple analogy, offered by Keane and Nair,[83] is that the space mapping approach is similar to drawing the low fidelity model on a rubberized sheet that can be then distorted to agree topologically with the high fidelity results. This seems to be a natural approach for solving inverse problems where the main objective is to find parameters of the model whereas a design optimization problem primarily aims at achieving the best performance characteristics (responses) of the system. This technique has been used extensively in microwave circuit design, see the review by Bandler et al.,[121] with fewer applications in other engineering fields. Leary et al.[122] demonstrated the use of space mapping in structural optimization on a simple beam problem. Ignatovich and Diaz[123] used space mapping in crashworthiness applications using a specially developed truss structure as a low fidelity model. Redhe and Nilsson[124] used a multipoint version of space mapping where a high fidelity response evaluation is done in each iteration to improve the mapping function and combined it with the response surface methodology. The technique is compared to the correction surface-based approach and applied to a vehicle crashworthiness structural optimization problem.

Until now, relatively little attention was paid to a case when the number of design variables in a low fidelity model differs from that in a high fidelity model, particularly when a different modeling concept is used, e.g., a 3D model is considered instead of a 2D model. In such cases some form of mapping between the spaces of the design variables is required. Robinson et al.[125] developed two new mapping methods, corrected space mapping and proper orthogonal decomposition (POD) mapping that are used in conjunction with trust region model management. It is reported that on a wing design problem the use of POD mapping achieved 53% savings in high fidelity function calls over optimization directly in the high fidelity space. In Robinson,[126] a hybrid between POD mapping and space mapping has been also developed and compared with the previously implemented techniques.

IV. Multiple Surrogates and Metamodel Ensembles

As outlined by Viana and Haftka,[80] the diversity of surrogate techniques is based primarily on a combination of three components:

1. The statistical model and its assumptions: for example, while response surface techniques assume that the data is noisy and the model obtained with the basis functions is exact, Kriging usually assumes that the data is exact but the function is a realization of a Gaussian process.
2. The basis functions: for response surfaces, the basis functions are usually monomials, but other functions have been occasionally used. Kriging allows different trend functions that are also usually monomials. In support vector regression, the basis functions are specified in terms of a kernel.
3. The loss function: while most surrogates are based on minimizing the root-mean-square error (RMSE), minimizing the average absolute error (L1 norm) leads to surrogates that are less sensitive to outliers. Figure 4 shows surrogates fitted to five data points. Four of them lie on a straight line and the fifth represents erroneous data. It is seen that while the erroneous point changes substantially the Kriging surrogate and a response surface based on RMSE, it has no effect on the fit based on the L1 norm.

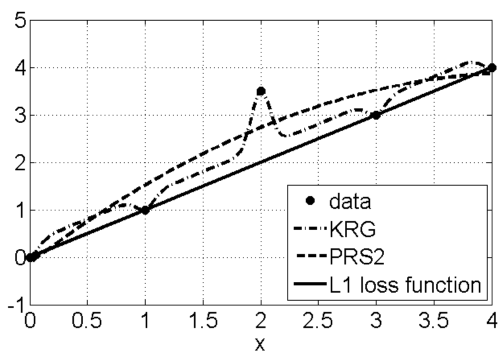


Figure 4. Differences of fitting due to different surrogate approaches (adopted from Ref. 81). Among 5 points sampled from a straight line, one presents a significant amount of error (x = 2 and y = 3.5). It can be seen that only L1 norm is not affected by this.

From the historical perspective discussed in Section II, the response surface and neural network literature has shown us that there are two issues when multiple models are to be considered: (i) selecting[127,128,129] and (ii) combining.[130,131] In both cases, everything starts with ranking the set according to a common criterion, which most of the time is an estimator of the RMSE known as PRESS (prediction sum of squares). PRESS is the mean square of the cross-validation errors. A cross-validation error is the error at a data point when the surrogate is fitted to a subset of the data points not including that point. When the surrogate is fitted to all the other $p - 1$ points, (so-called leave-one-out strategy), this process has to be repeated p times to obtain the vector of cross-validation errors, $\mathbf{e}$. Alternatively, the k-fold strategy can also be used for computation of the PRESS vector. According to the classical k-fold strategy,[132] after dividing the available data (p points) into p/k clusters, each fold is constructed using a point randomly selected (without replacement) from each of the clusters. Of the k folds, a single fold is retained as the validation data for testing the model, and the remaining k – 1 folds are used as training data. The cross-validation process is then repeated k times with each of the k folds used exactly once as validation data. Note that k-fold turns out to be the leave-one-out when $k = p$.

Selection based on PRESS is as simple as the straightforward use of the surrogate with the lowest PRESS. Exemplified by Roecker,[127] the literature on response surface shows the application of such approach for the selection of the coefficients of the polynomial. The same can be found in the neural network literature, Utans and Moody[128] applied the same concept for selecting neural network architectures.

Linear combination of different surrogates with weights defined according to the individual PRESS errors is also something that has been explored since long ago.[131] However, the advantages of combination over selection has never been clarified.[130] Viana and Haftka[133] recently pointed out that (i) the potential gains from using weighted surrogates diminish substantially in high dimensions, and (ii) the poor quality of the information given by the cross-validation errors in low dimensions makes the gain very difficult in practice. Having said that, a diverse set of surrogates can be obtained in practice by generating:

- Single instances of different metamodeling techniques: This is the more intuitive and straight forward approach, which often motivated by practical considerations. For instance, Mack et al.[134] employed polynomial response surfaces and radial basis neural networks to perform global sensitivity analysis and shape optimization of bluff body devices to facilitate mixing while minimizing the total pressure loss. They showed that due to small islands in the design space where mixing is very effective compared to the rest of the design space, it is difficult to use a single surrogate model to capture such local but critical features. Glaz et al.[135] used polynomial response surfaces, kriging, radial basis neural networks, and weighted average surrogate for helicopter rotor blade vibration reduction. Their results indicated that multiple surrogates can be used to locate low vibration designs which would be overlooked if only a single approximation method was employed. Samad et al.[136] used polynomial response surface, kriging, radial basis neural network, and weighted average surrogate in a compressor blade shape optimization of the NASA rotor 37. It was found that the most accurate surrogate did not always lead to the best design. This demonstrated that using multiple surrogates can improve the robustness of the optimization at a minimal computational cost.
- Multiple instances of same or different techniques: this is a less intuitive approach. Sanchez et al.[137] presented a approach toward the optimal use of multiple kernel-based approximations (support vector regression). They reported that in their set of analytical functions as well as in the engineering example of surrogate modeling of a field scale alkali-surfactant-polymer enhanced oil recovery process, the ensemble of surrogates, in general, outperformed the best individual surrogate and provided among the best predictions throughout the domains of interest. Viana and Hafka[133] studied whether to use the best PRESS solution or a weighted surrogate when a single surrogate is needed. They used a large set compound by 6 instances of kriging, 1 polynomial response surface, 1 radial basis neural network, and 16 instances of support vector regression. They found that (i) PRESS is good for ranking surrogates; and (ii) the limited gains (if any) of the weighted average surrogate makes it to act as an insurance against bad fitted surrogates.

As it turns out, the use of multiple surrogate (i.e., a set of surrogates and possibly a weighted average surrogate) is very appealing in design optimization due to the fact that the best surrogate may not lead to the best result; and complementary because fitting many surrogates and repeating optimizations is cheap compared to cost of simulation. Consider an optimization problem with 4 design variables and a single response. This would typically require 30 points for surrogate modeling. Say that each simulation runs in 30 minutes which implies in 7hs and 30min for sampling the design space. Let us compare two scenarios, one where we use a traditional polynomial response surface and another where in addition to that we also use 4 other more elaborated and expensive surrogates (such as kriging, neural networks or support vector regression). Let us consider the cost for PRESS calculation for all surrogates is 30 min. Table 2 shows the computational costs associated with running single point evaluation and optimization. It shows that the use of multiple surrogates for optimization is affordable when compared to the actual simulations. The total cost of using multiple surrogates involving sampling (most of the budget), PRESS computation and global optimization is an overnight operation. In this example, at the end of the optimization:

- If we use just the polynomial response surface, we end up with a single candidate solution that would require other extra 30min.
- If we use all 5 surrogate models, we end up with 5 candidate solutions that if we can not resume to a smaller set, it would require at most 2hs and 30min (in case of different solutions).

Table 2. Comparison of different exercises using actual and surrogate models.

Application	Number of evaluations	Actual model (4 variables, 1 response)	Single surrogate model	5 surrogate models
Extra point evaluation	1	30 min	0.05 sec	0.25 sec
Single-run optimization	500	10 days 10 hours	25 sec	2min 5 sec
Global optimization	10,000	208 days 8 hours	8min 30 sec	42 min 30 sec

V. Metamodeling Capabilities in Commercial Software

Developments in commercial software come from two primary sources: (1) academic research and (2) industrial needs. Academic research offers great flexibility and ability to explore different directions, whereas industrial needs are dictated by practical problems required to be solved in a short period of time. Software companies aim to accommodate current industry needs first (as their financing depends mostly on industry), but at the same time they try to anticipate any future needs in the industry. This necessity to anticipate future needs makes them conduct their own research and also requires them to pay attention to what is going on in academic research. Keeping the balance between efficient research for future needs and immediate day-to-day important industry requests is not an easy task, especially accounting for the need to sell the software. An essential part of this balance is efficient and robust implementation of the methods and algorithms. At the same time, although many methods in commercial software have similar names, the implementation is quite different due to different customer demands and needs as well as due to practical experience of software developers.

Currently there exists a number of commercial software that implements a variety of metamodeling techniques. However, one has to take into account that for many commercial software systems metamodeling is not an ultimate goal. Instead, in many cases metamodeling is a companion to optimization and design exploration capabilities, when identifying the best possible system for given conditions in an automatic fashion remains the main task.

The advances in computer technology and graphical user interface (GUI) development as well as conference presentations of competing software vendors led to a situation when quite a few commercial software systems offer similar capabilities regarding integration with the third party analysis/simulation codes as well as pre-/post-processing and even underlying algorithms. Even running on remote CPU's as well as parallel computation capabilities became a common feature of most of the software. As a result, on one hand the GUI aspects of various software products become resembling, on the other hand, similar algorithms may be called different names in different software. Learning curves for users may be different depending on the software environments. Because of all these factors, a potential user is strongly encouraged to talk to specific company regarding his/hers specific needs and personally evaluate several candidate software according to his/hers preferences: ease of use, typical computational cost for his/hers specific type of optimization problems, visualization capabilities, metamodeling and optimization algorithms, etc. to make sure that the software offers what is needed.

The same factors that force the user to spend more time evaluating each software (GUI similarity, similarity in post-processing and integration features, some fuzziness in the actual software capabilities, different names for similar algorithms, etc.) also make it harder to perform unbiased comparison of the software. The non-standardized terminology may be partially blamed for that (for example, from a user's prospective is there a difference between a "metamodel" and an "approximation"?). But the main reason being that for majority of software companies selling software became a necessity with all its pluses (the need to develop fast and robust algorithms along with nice companion capabilities) and minuses (the need to actually sell the product, rather than to just periodically present papers with detailed description of all its capabilities, updates, and new applications.)

Table 3 lists some of the popular commercial software products and their capabilities related to metamodeling methods and general-purpose optimization. The software products are presented in alphabetical order. We present neither a complete list of all available software products, nor the complete list of capabilities, but rather, a brief introduction to software available specifically for metamodeling and optimization tasks. The table is followed by some remarks regarding each of the software. We did not include popular software (e.g., MATLAB,[‡‡] Excel,[§§] JMP,[***] Minitab[†††]) that do not specialize in optimization into the table; however, we do provide some remarks regarding their capabilities.

- BOSS/Quattro: It is an application manager that offers an easily customizable environment with native driver files for major CAD/CAE, FEA, MBS and CFD software, including managing sensitivities. BOSS/Quattro:may also use XML formalism.
- Dakota: It is a public domain software. Being more driven by research and publications, it tends to be more on the leading edge of the algorithms than the commercial software. Dakota has more variety of optimization and metamodeling methods than commercial software. However, because of the lack of demanding paying customers the user-friendliness is less than in commercial software. Specifically, inexperienced users may be overwhelmed by a variety of algorithms and options in each of them. Use of C++ as a core language, provides plug-and-play capability of components and natural paths for extendability. Having several thousands of

[‡‡] www.mathworks.com
[§§] office.microsoft.com/en-us/excel
[***] www.jmp.com
[†††] www.minitab.com

download registrations from around the world, Dakota relies on community discussion forums to enable a distributed support model. This is different from the commercial model and requires some sophistication from the user base to be able to function without commercial-quality support.

Table 3. Commercial software metamodeling and optimization capabilities.

Software Product	Metamodeling Capabilities	Optimization Capabilities
BOSS/Quattro (SAMTECH S.A) www.samcef.com	Least Squares Regression for Polynomials and Posynomials, Radial-Basis Functions, Neural Networks, Kriging	Gradient-based optimization, Surrogate-based optimization, Genetic Algorithm, Multiobjective optimization, Probabilistic optimization
Dakota (Sandia National Laboratories) www.cs.sandia.gov/DAKOTA	Taylor Series Approximation, Least Squares Regression for Polynomials, Moving Least Squares, Neural networks, Kriging, Radial-Basis Functions, Multipoint Approximations, multifidelity modeling, Multivariate Adaptive Regression Splines (MARS)	Large variety of methods, including Surrogate-based optimization, Gradient-based optimization, Evolutionary optimization, Multiobjective, Probabilistic optimization
HyperStudy (Altair Engineering) www.altair.com	Least Squares Regression for Polynomials, Moving Least Squares Method for Polynomials, Kriging	Surrogate-based optimization, Gradient-based optimization, Genetic Algorithm, Probabilistic Optimization
IOSO (Sigma Technology) www.iosotech.com		Self-organizing optimization algorithms specifically targeted for multiobjective and probabilistic optimization
iSight (Dassault Systemes, formerly - Engineous Software) www.engineous.com	Least Squares Regression for Polynomials, Taylor Series Approximation, Radial-Basis Functions, Neural Networks, Kriging, variable-complexity modeling	Surrogate-based optimization, Gradient-based optimization, Genetic Algorithm, Simulated Annealing, Probabilistic Optimization, Multiobjective optimization
modeFRONTIER (Esteco) www.esteco.it	Least Squares Regression for Polynomials, K-Nearest interpolation, Kriging, Bayesian Regression, Neural networks	Surrogate-based optimization, Gradient-based optimization, Genetic Algorithm, Simulated Annealing, Particle Swarm Optimization, Evolution Strategies, Probabilistic Optimization, Multiobjective optimization
Model Center (Phoenix Integration) www.phoenix-int.com	Least Squares Regression for Polynomials	Gradient-based optimization, Genetic Algorithm
OPTIMUS (Noesis Solutions) www.noesissolutions.com	Least Squares Regression for Polynomials, Radial-Basis Functions, Kriging, User-defined models, AIC methodology to find model terms	Surrogate-based optimization, Gradient-based optimization, Differential Evolution, Self-adaptive Evolution, Simulated Annealing, Probabilistic Optimization, Multiobjective optimization, User-defined optimzer
VisualDOC (Vanderplaats Research and Development, Inc.) www.vrand.com	Least Squares Regression for Polynomials	Surrogate-based optimization, Gradient-based optimization, Genetic Algorithm, Particle Swarm Optimization, Probabilistic Optimization, Multiobjective optimization

- Excel: Not widely known is the fact that Excel has an optimization tool suitable for solving non-linear problems. Although lagging behind specialized optimization software in terms of the scale of problems that can be solved, Excel Solver provides nice and easy to use optimization capabilities. In addition to that, most of the commercial optimization/metamodeling software packages have specialized interfaces to Excel.
- HyperStudy: One of the main advantages of the software is its close ties to the other products by Altair Engineering, especially to HyperMesh - a popular pre-post-processor for major CAD/CAE, FEA, and CFD software. The integration with HyperMesh enables direct parameterization of FEA/MBD/CFD solver input data and one-step extraction of plot and animation output, thus making the solver integration to HyperStudy efficient. Shape variables can be easily defined using the morphing technology in HyperMesh without the need

for CAD data. Advanced data mining techniques in HyperStudy such as redundancy analysis and clustering with principal component analysis simplifies the task of studying, sorting and analyzing results.

- IOSO: IOSO offers unique state of the art optimization algorithms that are based on self-organizational strategy and efficiently combine traditional response surface methodology with gradient-based optimization and evolutionary algorithms in a single run. The offered algorithms are equally efficient for the problems of complex and simple topology that may include mixed types of variables.
- iSight: iSight is one of the most widely used commercial optimization packages. It supports direct integration to a large number of third party analysis/simulation tools and CAD programs. One of the unique iSight tools offers using the physical dimensions of the parameters to create a smaller number of non-dimensional parameters for easier and semi-automatic reduction of the design variables and identifying underlying trends in system designs. iSight is tightly coupled with the plug-and play-engineering workflow environment based on the FIPER architecture, which allows workflow and component sharing as well as web workflow execution.
- JMP: Although lacking the direct optimization capabilities, JMP and SAS software are definitely worth to be aware of, as this software is the leader and de-facto a standard in statistical analysis, design of experiments technique, and response surface modeling.
- MATLAB: MATLAB's main focus is not metamodeling or optimization. Rather, it is a numerical computing environment and programming language. It is a flexible and wide spread tool with almost all specialized metamodeling/optimization software having direct interfaces to it. In addition, MATLAB itself has an optimization/metamodeling tool box with a variety of algorithms and options available. As MATLAB provides nice programming, pre- and post –processing capabilities as well as links, methods, and tools from a wide variety of fields, it is in itself an attractive system for optimization and metamodleing.
- Minitab: Like JMP, Minitab lacks direct optimization capabilities. However, being one of the most popular statistical packages, Minitab certainly is one of the leaders in generating and performing statistical analysis on various metamodels.
- modeFRONTIER: modeFRONTIER is used in a wide range of applications across all industry sectors, but prides itself in advanced engineering fields that use CAE packages. modeFRONTIER provides a range of intuitive yet impressive and powerful data visualization and data filtering tools and charts. Along with a range of statistical data analysis tools, it also offers multidimensional analysis and clustering methods such as Self Organizing Maps, Hierarchical and Partitive clustering.
- Model Center: The main focus of Phoenix Integration is integration of various software into a single design environment, when software models can be located across the network or locally. Model Center has specific tight interfaces to many analysis/simulation software from various fields. Optimization is viewed as just one part of this environment. Third party optimizers may be plugged into this environment.
- OPTIMUS: In addition to offering optimization procedures, and specialized interface to many CAD/CAE packages and local "legacy" codes, OPTIMUS automates and monitors simulation processes as well as allows the users to automatically visualize and explore the design space. OPTIMUS automates simulation tasks across multiple engineering disciplines and offers more flexibility for process integration by allowing multiple nested workflows. One of the unique features of OPTIMUS is linking user's own optimizer with OPTIMUS.
- VisualDOC: With development led by Dr. Garret N. Vanderplaats, VisualDOC offers a simple and intuitive, but robust and flexible environment for interfacing with any analysis/simulation software to efficiently solve any general-purpose optimization problem. The main distinction of VisualDOC is one of the most efficient and robust gradient-based optimization algorithms. VisualDOC offers real-time "what-if" post-process study tool and provides C/C++ API that allows embedding all its capabilities inside of the third party program.

VI. Metamodel-Driven Design Space Exploration and Visualization

Metamodeling not only reduces the computational costs of optimization but also provides a means for rapid design space exploration and, more importantly, visualization. Because metamodels are approximations, they are fast, virtually instantaneous, which enables performance analyses to be computed in real-time when design (input) variables are changed within a graphical design environment. The importance of having fast response in graphical design interfaces has been corroborated by many studies. Nearly thirty years ago, Goodman and Spence[138] found that response delays as little as 1.5 seconds in the software can increase task completion time by approximately 50%. Recent experimental studies have found similar results: task completion times increased by 33% when response delays were 1.5 seconds.[139] These recent studies have also found that errors in user performance – the ability to locate the optimum within the design interface – can increase by 150%[140] or nearly twice that amount[139] when response delays are 1.5 seconds are present, depending on the size and complexity of the problem. Needless to say, rapid analysis capability for effective design space exploration is paramount in today's computer-mediated design environment.

Within the MDO community, research in this area has proceeded primarily in two fronts: (1) improving software and visualization tools that use metamodels for design space exploration, and (2) assessment of visualization strategies that employ metamodels. Examples of the former include Graph Morphing,[141,142] Cloud Visualization,[143] Brick Viz,[144] and the Advanced Systems Design Suite,[145,146] which utilize metamodels of various types to allow users to steer and visualize a simulation through real-time interactions. Recent developments have sought to improve methods for visualizing the resulting n-dimensional Pareto frontiers.[147,148] Meanwhile, aerospace researchers at Georgia Tech have been extensively utilizing the metamodeling and visualization capabilities in JMP to perform multi-dimensional trade studies and explore the design space.[40,149] Ford Motor Company and SGI also joined forces to investigate the use of surrogate modeling and high performance computing to facilitate rapid visualization of design alternatives during the MDO process.[150] Finally, researchers at Penn State and the Applied Research Laboratory are investigating the use of visual steering commands that allow designers to explore and navigate multi-dimensional trade spaces in real-time using the rapid analysis capabilities of metamodels.[151,152]

As for the second line of research, assessment of the benefits of metamodel-based visualization is becoming more prevalent now that visual design environments are routinely used by many engineering design teams. For instance, Ligetti and Simpson[153] studied the use of first-order, stepwise, and second-order polynomial regression models for approximating the system responses in a detailed manufacturing simulation and found that using stepwise regression models significantly reduced task completion time and decreased error compared to the first-order and second-order polynomial regression models. These improvements in efficiency and effectiveness, respectively, resulted primarily from having a more parsimonious regression model (i.e., the same level of accuracy with the fewest possible terms) during the one-factor-at-a-time variations that were permitted within the graphical design interface. Meanwhile, in a wing design problem that used second-order response surface models for analysis, Simpson et al.[140] found that problem size significantly affected the users' average error, which doubled each time as it increased from two to four and then to six design variables. These findings, in combination with the aforementioned importance of response delay, have significant implications on the use and development of metamodel-driven visual design environments – the potential benefits are great, but we must be very mindful of the human-computer interaction to avoid the pitfalls that can likewise occur.

VII. Summary and Conclusions

In this paper, we examined the advancements in the design and analysis of computer experiments (DACE) within the MDO community in the past twenty years. We begin with a historical perspective to better understand the extent to which the use of metamodeling techniques in MDO have evolved in the two decades since the seminal paper on Design and Analysis of Computer Experiments by Sacks et al.[1] Based on current thrusts in the field, we delve deeper into multi-level and multi-fidelity approximations and ensembles of metamodels, as well as the availability of metamodels within commercial software and for design space exploration and visualization.

The goal in the paper has been to better understand how developments in DACE are being used today while providing a collection of relevant references that the complement existing literature reviews. We are also happy to see that books about DACE, written by engineers for engineers, are finally starting to appear.[154] These and related efforts (e.g., freely available surrogate toolboxes for the widely-used Matlab[‡‡‡]) will continue to broaden the use of DACE in MDO and non-MDO arenas while fostering its acceptance by an even larger community.

In closing, while DACE is becoming more mainstream, the majority of the research challenges remain the same:

- *Curse of dimensionality*: still exists – the problems have just gotten larger
- *Computational complexity*: still exists – problems have just gotten more complex and/or we are trying to do more (e.g., robust design, OUU, RBDO)
- *Issues with numerical noise*: still exists and may have gotten worse due to added computational complexity of many analyses
- *Challenges with handling mixed discrete/continuous variables*: still exits, and also may have gotten worse due to the nature of problems now being investigated
- *Validation of metamodel and the underlying model*: still also critical as before but now incorporating the error of the underlying model itself into the problem formulation is becoming more important.

[‡‡‡] For instance, see the DACE Matlab Kriging Toolbox (http://www2.imm.dtu.dk/~hbn/dace/) and the more general surrogate modeling toolboxes (http://fchegury.110mb.com/surrogatestoolbox.htm).

The main learning from this paper is that although the big picture may mislead one to conclude that the computational budget is the main motivation behind the research on DACE, a closer look reveals that the demand for new and tougher capabilities is what really pushes the developments. We hope that this work can help both new and experienced researches to situate and to get inspired by the advances in the DACE research.

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