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Approximation methods in multidisciplinary analysis and optimization: a panel discussion*

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Abstract This paper summarizes the discussion at the *Approximation Methods Panel* that was held at the *9th AIAA/ISSMO Symposium on Multidisciplinary Analysis & Optimization* in Atlanta, GA on September 2–4, 2002. The objective of the panel was to discuss the current state-of-the-art of approximation methods and identify future research directions important to the community. The panel consisted of five representatives from industry and government: (1) Andrew J. Booker from The Boeing Company, (2) Dipankar Ghosh from Vanderplaats Research & Development, (3) Anthony A. Giunta from Sandia National Laboratories, (4) Patrick N. Koch from Engineous Software, Inc., and (5) Ren-Jye Yang from Ford Motor Company. Each panelist was asked to (i) give one or two brief examples of typical uses of approximation methods by his company, (ii) describe the current state-of-the-art of these methods used by his company, (iii) describe the current challenges in the use and adoption of approximation methods within his company, and (iv) identify future research directions in approximation methods. Several common themes arose from the discussion, including differentiating between design of experiments and design and analysis of computer experiments, visualizing experimental results and data from approximation models, capturing uncertainty with approximation methods, and handling problems with large numbers of variables. These are discussed in turn along with the future directions identified by the panelists, which emphasized educating engineers in using approximation methods.

Key words analysis of variance, approximation methods, design of experiments, kriging, response surfaces, surrogate models

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1 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. For instance, Ford Motor Company reports that one crash simulation on a full passenger car takes 36–160 hours (Gu 2001). The high computational expense of such analyses limits, or often prohibits, the use of such codes in engineering design and multidisciplinary design optimization (MDO). 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. The basic approach is to construct a simplified mathematical approximation of the computationally expensive simulation and analysis code, which is then used in place of the original code to facilitate multidisciplinary design optimization, design space exploration, reliability analysis, etc. Since the approximation model acts as a *surrogate* for the original code, it is often referred to as a surrogate model, surrogate approximation, approximation model, or metamodel (i.e. a "model of a model" (Kleijnen 1975)). A variety of approximation models exist (e.g. polynomial response surfaces, kriging models, radial basis functions, neural networks, multivariate adaptive regression splines), and recent reviews and comparisons of many of these approximation model types can be found in (Simpson *et al.* 2001b,c; Jin *et al.* 2001; Sobieszczanski-Sobieski and Haftka 1997; Haftka *et al.* 1998; Barthelemy and Haftka 1993; Barton 1998).

To gain a better understanding of how approximation methods are currently viewed and being used by industry and government agencies, a panel discussion on *Approximation Methods* was held at the *9th AIAA/ISSMO Symposium on Multidisciplinary Analysis & Optimization* (MA&O) in Atlanta, GA on September 2–4, 2002. The objective of the panel was to discuss the current state-of-the-art of approximation methods and identify future research directions important to the community. The panel consisted of five representatives from industry and government: (1) Andrew J. Booker from The Boeing Company, (2) Dipankar Ghosh from Vanderplaats Research & Development, (3) Anthony A. Giunta from Sandia National Laboratories, (4) Patrick N. Koch from Engineous Software, Inc., and (5) Ren-Jye Yang from Ford Motor Company. Each panelist was asked to (i) give one or two brief examples of typical uses of approximation methods by his company, (ii) describe the current state-of-the-art of these methods used by his company, (iii) describe the current challenges in the use and adoption of approximation methods within his company, and (iv) identify future research directions in approximation methods.

The remainder of this paper summarizes the discussion that occurred at the panel and is intended to serve as a record for the approximation methods community at large who were unable to attend. Section 2 covers discussion points (i) and (ii). It contains a brief overview of the example applications discussed by the panelists along with a list of the approximation software presented during the panel, which represents the state-of-the-art at each company. Several common themes arose from discussion points (iii) and (iv), and these included differentiating between design of experiments and design and analysis of computer experiments (Sect. 3), visualizing experimental results and data from approximation models (Sect. 4), capturing uncertainty with approximation methods (Sect. 5), and handling problems with large numbers of variables (Sect. 6). A brief summary of the questions that followed the panelists' opening remarks are discussed as part of the closing remarks in Sect. 7 along with future challenges such as educating engineers in using approximation methods.

2 Overview of applications of approximation methods

A variety of applications were discussed by the panelists, indicating the wide variety of uses for approximation methods in engineering design and MDO. These applications ranged from space station power systems, to fluid flow problems and oil tanker design, to structural design and automotive crashworthiness. A brief overview of each example follows.

Booker described a design of experiments approach that was used to verify the performance of large DC power systems for a space station (Karimi *et al.* 1996, 1997). Between 10 and 30 input loads could be switched ON/OFF, and Design of Experiments was used to analyse the performance of the system and determine operating conditions to achieve a desired phase margin. Since each load could be switched either ON or OFF, a two-level, resolution V fractional factorial design was used to analyse the system (128 runs for the 10-variable case, 1024 runs for the 30-variable case), and analysis of variance (ANOVA) was used to estimate main effects. Additional experiments on subsets of the variables were used to confirm the optimum point determined from the approximation.

Booker also discussed an aircraft jet engine inlet design problem involving 11 geometry parameters and five responses that used a 12-pt Plackett–Burman design (Plackett and Burman 1946) to achieve an accurate approximation to maximize the airflow rate on the inlet surface (Mason *et al.* 1992). The design was subsequently successively augmented by "folding over" the design to resolve interactions and adding a centre point and star points to estimate quadratic effects, yielding a total of 23 runs (12-pt Plackett–Burman design $+5 \times 2$ star points $+1$ centre point). The peak Mach number on the inlet surface was estimated at five flight conditions and compared to linear and quadratic model predictions; details can be found in Mason *et al.* (1992). The significance of this example was not so much the improvement in the design, but the fact that the initial turnaround time of two weeks for the analyses was reduced to one day by automating the set-up to run the experiments. The benefit of the particular experimental design approach on this problem was the ability to augment sequentially the design as turnaround time was reduced.

A fluid flow example involving the design of a cooling system (Quinn 2002) was presented by Ghosh during the panel, see Fig. 1. The example consisted of 12 design variables, 10 constraints, and one objective function; feasibility and convergence were achieved in 11 iterations, requiring only 24 calls of Fluent, a computationally expensive fluid flow analysis software program. The approximation model was successful in helping find a feasible final solution since the initial solution was infeasible; the optimum design was then determined directly in Fluent.

Koch discussed an oil tanker conceptual design problem from (Golovidov *et al.* 1999) that was used to com-

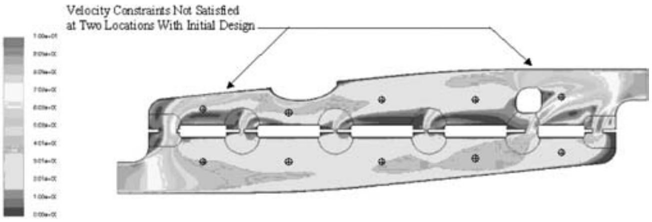


Fig. 1 Visualization of fluid flow through cooling system using Fluent

pare the accuracy of a single global approximation model against two disciplinary analysis models – one for the tanker's hydrodynamic analyses and one for the tanker's structural analyses – that provided parameters for cost estimation. The global response surface model had six inputs, 14 outputs, and required 50 function evaluations of each of the actual codes (i.e. hydrodynamic and structural analyses) to build the global approximation model. For the individual disciplinary approximations, only 25 function evaluations were required to build approximations of the four inputs and seven outputs for the hydrodynamic analyses, which were combined with a sequentially updated Taylor-series approximation (53 evaluations total) of the structural analysis. The global approximation yielded a feasible tanker design with a return on investment (ROI) of 1.118 while the combined two disciplinary approximations yielded a feasible design with a ROI of 1.114; both designs are improvements over the initial design, which is highly infeasible and had a scaled ROI of 1.0. Both solutions from the approximations were accurate to within 0.05 of the actual objective function even though the individual approximations used fewer function evaluations.

Approximation methods for structural analysis and automotive crashworthiness were discussed by several panelists. Yang described an automobile design example involving the use of topology optimization to improve the structural rigidity of the body (Leiva *et al.* 2001). Vehicle safety analysis is a complex and computationally expensive process, and researchers at Ford are investigating the accuracy of different approximation types for automotive crashworthiness studies (Gu 2001; Yang *et al.* 2000, 2001). Yang *et al.* (2001) stress the importance of uniform sampling when only small sets of sample points are available due the computational expense of running crash simulations such as that shown in Fig. 2(a). This example had nine input variables, 11 output responses, and used only 33 points to fit global models to analyse crashworthiness. Meanwhile, a probabilistic formulation for addressing uncertainty in automotive design was presented by Koch to help identify designs that are robust to the crash scenarios (see Fig. 2(b)) that are considered during automotive crashworthiness studies (Koch *et al.* 2004; Koch and Gu 2001; Yang *et al.* 2002).

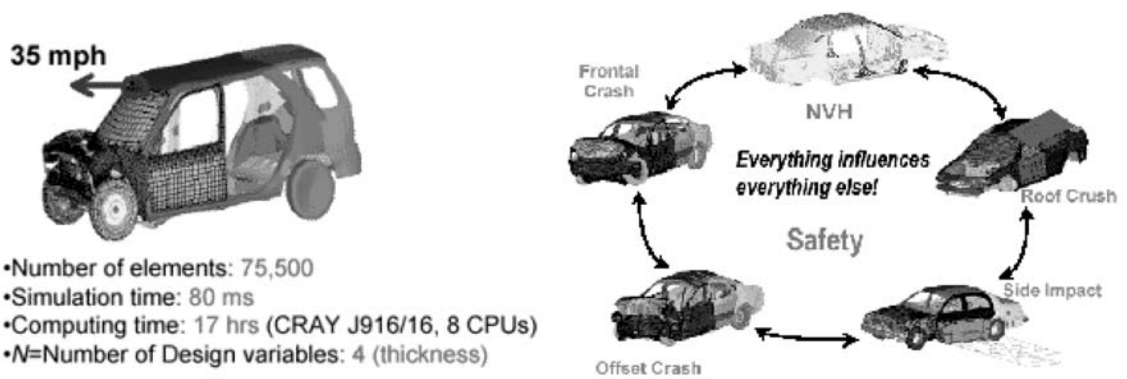
In addition to these examples, several software packages for building, constructing, validating, and optimizing approximation models were discussed by the panelists. To avoid commercialism and bias, the reader is referred to the following references and URLs to learn more about the capabilities of the approximation software packages discussed by the panelists:

– DAKOTA (Eldred *et al.* 2002a:)
  `http://endo.sandia.gov/DAKOTA`.
– iSIGHT (Koch *et al.* 2002b):
  `http://www.engineous.com/products.htm`.
– VisualDOC (Balabanov *et al.* 2002):
  `http://www.vrand.com/visualdoc3info.htm`.

In addition to these packages, Design Explorer is being developed at The Boeing Company to provide similar capabilities (Booker *et al.* 1999).

3 Challenge 1: Design of experiments versus design and analysis of computer experiments

As mentioned previously, several common themes arose from the panel discussion, including the need to differentiate between design and analysis of computer experi-



(a) Example Front Impact Simulation (b) Analyses Involved in Crashworthiness Study

Fig. 2 Automotive crashworthiness

ments (DACE) and what we will term here "traditional response surface methods". There is an important distinction between physical experiments, which have random error, and computer experiments, which are often deterministic (i.e. the same output is obtained each time the same input is given), which was made frequently during the panel. Traditional response surface methods, as discussed in Box and Draper (1987), assume that experiments have sources of stochastic error, i.e. noise. They typically assume the response function being modelled is a polynomial. This is based on the assumption that the independent variables are being varied in a small enough region so that a Taylor expansion is appropriate. In contrast, DACE, as discussed in Sacks *et al.* (1989), assumes responses are deterministic and makes only continuity or levels of differentiability assumptions about the response being modelled (see Fig. 3). A recent overview of experimental design methods for computational simulations can be found in Giunta *et al.* (2003). The next two paragraphs describe how the underlying assumptions in the two methods impact the choice of appropriate experimental designs.

Traditional response surface methods were originally developed for design and analysis of physical experiments (Box and Draper 1959) where sources of random variation must be accounted for by randomization, by blocking, by spreading the sample points out in the design space, and by taking multiple data points (replicates) as shown in Fig. 3. The design of an experiment for traditional response surface methods will also ensure that coefficients in a polynomial model are estimated in an "orthogonal" (statistically independent) as possible way by accounting for confounding or aliasing in the experiment. So for example, two-level fractional factorial designs for polynomials with linear and cross terms (Box *et al.* 1978) are constructed with sufficient "resolution" to ensure that cross (interaction) terms can be estimated without having the estimates influenced by the presence of linear terms. Another example is the very important feature of central composite designs (Box and Draper 1987) for second-order polynomials that are typically "blocked" to allow one to, for example, do half the experiment on one day (block 1), and another half on a second day (block 2).

Sacks *et al.* (1989) state that the "classical" notions of blocking, replication, and randomization are irrelevant when it comes to deterministic computer experiments. In addition, very little is known a priori about the shape of the response function. Thus, one could argue, sample points should be chosen to fill the design space. Space

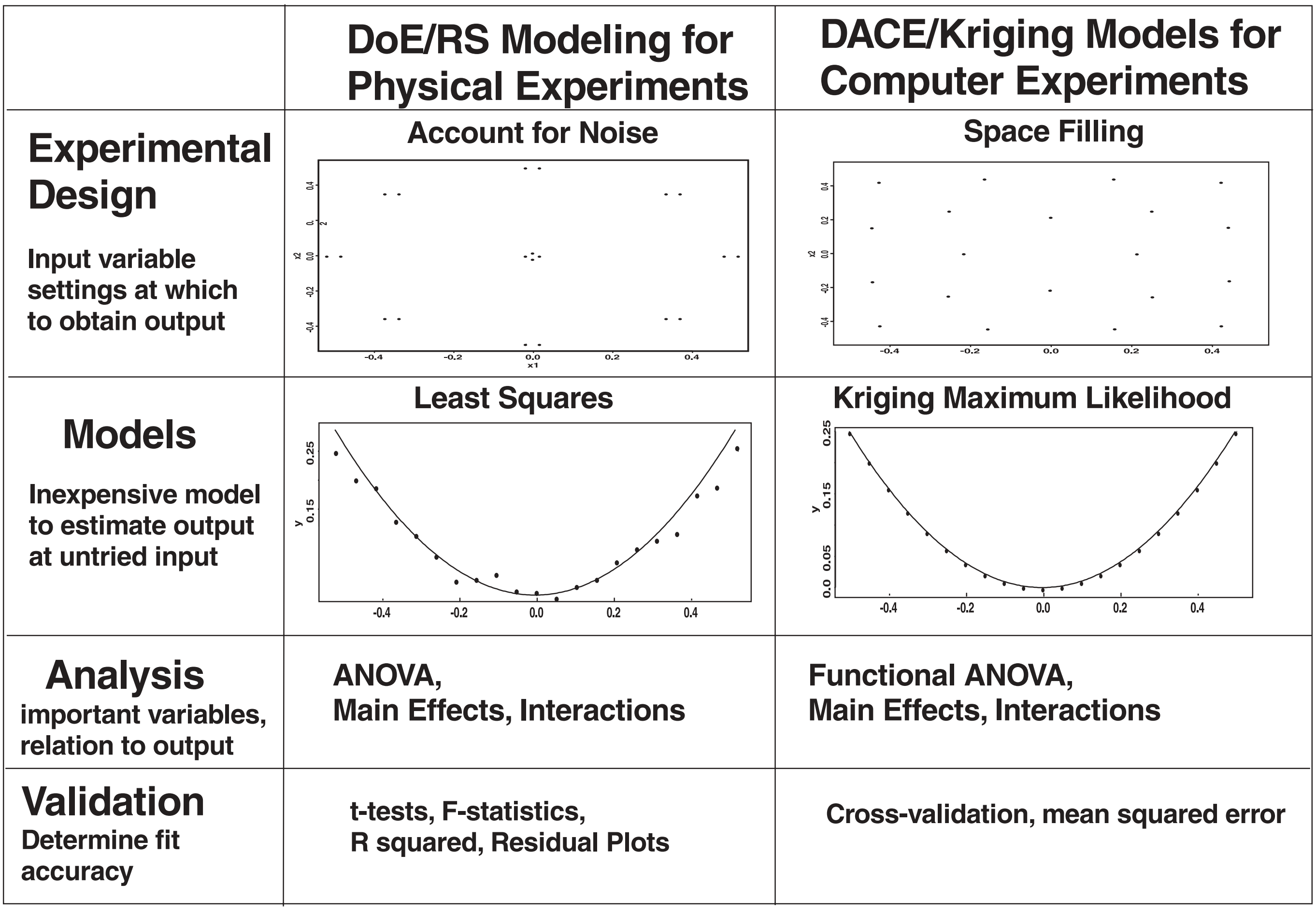


Fig. 3 Comparison of DOE/RS and DACE/Kriging (Booker 1998)

filling experimental designs include Latin hypercube designs (McKay *et al.* 1979), orthogonal arrays (Hedayat *et al.* 1999; Owen 1992), uniform designs (Fang and Wang 1994; Fang *et al.* 2000), Hammersley sampling sequences (Kalagnanam and Diwekar 1997), and minimax and maximin designs (Johnson *et al.* 1990) to name a few[1,2]. We note that one "experimental design" part of traditional response surface methods, i.e. confounding or aliasing, can be a very useful concept in deterministic experiments and was the motivation for using these methods in the power system example and engine inlet example. These notions are somewhat accounted for in Latin hypercube designs and orthogonal arrays via "strength" (Owen 1992). Note also that one could use space-filling designs and fit traditional polynomial response surfaces to the results as many researchers have done.

A class of designs that may bridge traditional response surface methods and deterministic computer experiments is "optimal designs". A complete discussion is beyond the scope of this paper. We note that so-called "alphabetic optimal designs" (Box and Draper 1987), A-, D- and G-optimal, exist in the context of traditional experiments (Box and Draper 1987) and in deterministic computer experiments (Sacks *et al.* 1989; Johnson *et al.* 1990). Roughly speaking, these designs attempt to choose points by minimization of some measure of error in prediction, based on an underlying assumed model. Another type of optimal design is a "minimum bias design" (see e.g. Box and Draper 1987, pages 437–442) that attempts to choose points for fitting a particular model given a model for the departure of the "true" response from the model being fit. Minimum bias designs may be in some sense "space filling", depending on the assumed model for the departure. The main difficulty with optimal designs is their calculation, especially for large problems, and the added difficulty of specification of an "assumed departure" for minimum bias designs. A notable exception is in Welch (1983) in which very little is assumed about the underlying "true" model.

Once sample data has been gathered, traditional response surface modelling typically employs least-squares regression to fit a polynomial model, typically first- or second-order, to the sampled data so that it captures the trends within the noisy data (see Fig. 3). Additional details on least-squares regression can be found in a number of texts (Myers and Montgomery 1995; Box and Draper 1987; Box *et al.* 1978). Kriging models are constructed using maximum likelihood estimation (see e.g. Sacks *et al.* 1989; Booker 1998; Currin *et al.* 1991; Koehler and Owen 1996; Giunta and Watson 1998; Simpson *et al.* 2001a), and typically interpolate the data, providing an exact fit of the sampled data. Non-interpolative kriging models that "smooth" noisy data can also be developed (Cressie 1988; Montès 1994; Kleijnen and Van Beers 2003).

Once the approximation model is constructed, it must be validated in order to ensure that it is sufficiently accurate to use as a surrogate for the original code. Validation of response surface models is typically based on: (a) testing statistical hypothesis (t-tests and F-statistics) derived from error estimates of the variability in the data, (b) plotting and checking the residuals, and (c) computing R^2, the ratio of the model sum of squares to the total sum of squares, and ${R^2}_{adj}$, which is R^2 adjusted for the number of parameters in the model (Myers and Montgomery 1995). Jin *et al.* (2001) discuss multiple performance metrics for comparing approximation models based on accuracy, efficiency, robustness, model transparency, and simplicity; Yang added that Gearhart and Wang (2001) discusses metrics for comparing response surface models of different order to identify the "best" model.

Sacks *et al.* (1989) and Welch *et al.* (1990) state that statistical testing is inappropriate when it comes to deterministic computer experiments which lack random error; therefore, cross-validation and mean-square error (MSE) are often employed to assess the accuracy of a kriging model. A simplified procedure for leave-one-out cross validation of kriging models is presented by Mitchell and Morris (1992), but recent studies by Meckesheimer *et al.* (2002) found that leave-one-out cross validation does not work well for validating kriging models. Leave-one-out cross validation often underestimates the true root-mean-square error in a kriging model, and they suggest using the more general leave-k-out cross validation for kriging models with $k = 0.1n$ or $\sqrt{n}$ where n is the number of sample points used to fit the model.

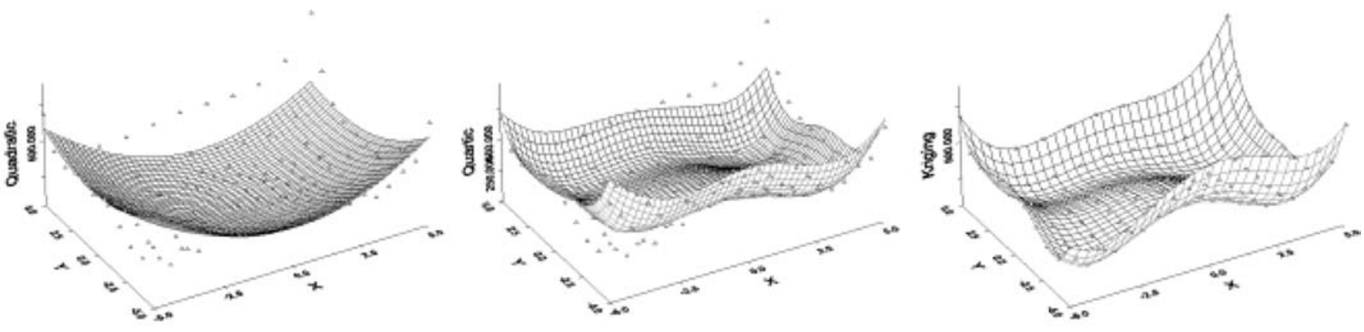
4
Challenge 2: Visualizing experimental results and data from approximation models

The importance of visualization was stressed by nearly every panelist. First, visualization is useful for examining the experimental results themselves and can be used to detect potential outliers in the data. Booker described a case were an errant run of a simulation code yielded a response about 10^6 orders of magnitude greater than the other responses, which caused the resulting kriging approximation to fit poorly. The engineers had not noticed the outlier when they examined the experimental data file, but it showed up immediately when the design space was plotted in 3D.

In addition to viewing the experimental results, approximation models also provide a useful surrogate for visualizing the entire design space. Koch gave the example shown in Fig. 4 of three approximation models fit to the same set of sample data – all three can be used to view

[1] The orthogonal arrays mentioned here are not limited to "Taguchi" orthogonal arrays and thus are not typically discussed in the traditional response surface literature. A notable exception is (Hamada and Wu 2000).

[2] A recent comparison of several space filling designs can be found in Simpson *et al.* (2001c).



(a) 2nd Order RS Model (b) 4th Order RS Model (c)Kriging Model

Fig. 4 Graphical comparison of response surface and kriging model

the design space, but which is the most accurate? Based on the sample data (indicated by small triangles in the figure) the design space is highly nonlinear, and it cannot be accurately represented by a second-order RS model as seen in Fig. 4(a). Higher-order polynomials are possible with the given data or multiple models could be fit over the design space; however, the plots in Fig. 4 are used to compare global models of the most commonly used response surface polynomials to the kriging model fit. A fourth-order RS model is shown in Fig. 4(b) fit to the sample data, but the symmetric fourth-order RS model does not capture the asymmetry of the underlying function. The kriging model shown in Fig. 4(c) provides the best fit to the sample data; it interpolates the sample data and has sufficient flexibility to model the highly nonlinear design space. A detailed example of a graphical comparison of response surface and kriging models for the design of an aerospike rocket nozzle can be found in Simpson *et al.* (2001a).

Visualization also plays an important role in optimization. Ghosh stressed the importance of viewing the history of the objective function during optimization to monitor system performance. Koch advocated using the approximation model to view design variable values in real-time as they changed during optimization. Booker stated that visualization is helpful in understanding why a point is optimum and how it might be improved if constraints are changed or relaxed.

Panelists also emphasized that these visualization capabilities do not have to be very sophisticated. Booker uses bar charts and pie charts to display functional ANOVA results to help identify important main effects and interactions based on the sample data (Karimi *et al.* 1997; Booker 1998, 2000a). Depending on the type of experimental design, the functional ANOVA can be computed directly, if using an orthogonal array of strength 3 or higher (Owen 1992), or can be estimated from the approximation model itself. Booker showed results from a sinusoidal test function proposed by Giunta and Watson (1998) to demonstrate the useful information that could be gained through functional ANOVA but with some caution when using approximate models to estimate the ANOVA (Booker 2000a).

5 Challenge 3: Capturing uncertainty with approximation methods

Approximation methods are becoming popular tools for modelling uncertainty and reducing the computational expense of probabilistic analysis during probabilistic design optimization. Koch stated that a variety of probabilistic methods have been developed to model and assess the effects of known uncertainties by converting deterministic problem formulations into probabilistic formulations, but until recently the computational expense of probabilistic *analysis* of a given design often precluded its application to real engineering design problems, and probabilistic *optimization* has thus been considered impractical, particularly for complex multidisciplinary problems. He stated that approximation methods are finding new uses in reducing the computational expensive of probabilistic analysis to make probabilistic optimization more tractable. Approximation models are being used at Ford to incorporate uncertainty into automotive crashworthiness studies (Koch *et al.* 2004; Koch and Gu 2001; Yang *et al.* 2002). Koch also outlined a procedure for using approximation methods to facilitate reliability analysis and robust design optimization, see Fig. 5. As an example, the oil tanker example described in Sect. 2 was used to compare the performance of response surface and kriging approximations for six-sigma-based probabilistic design optimization in Koch *et al.* (2002a).

Giunta used the plot in Fig. 6 to illustrate the differences between a global non-robust optimum and a local robust optimum. Figure 6 was produced in a computational shock physics application that employed a finite element code to simulate the implosion of an inertial confinement fusion capsule (Giunta *et al.* 2002). In this capsule design study, the goal was to obtain high implosion velocity and insensitivity to manufacturing variations of ± 0.005 cm on the capsule ablator radius, where the radius varied from 0.101 cm to 0.104 cm. Giunta stated that for this design problem it was more important to find robust, "flat" regions in the design space that were insensitive to these variations than it was to find the global optimum.

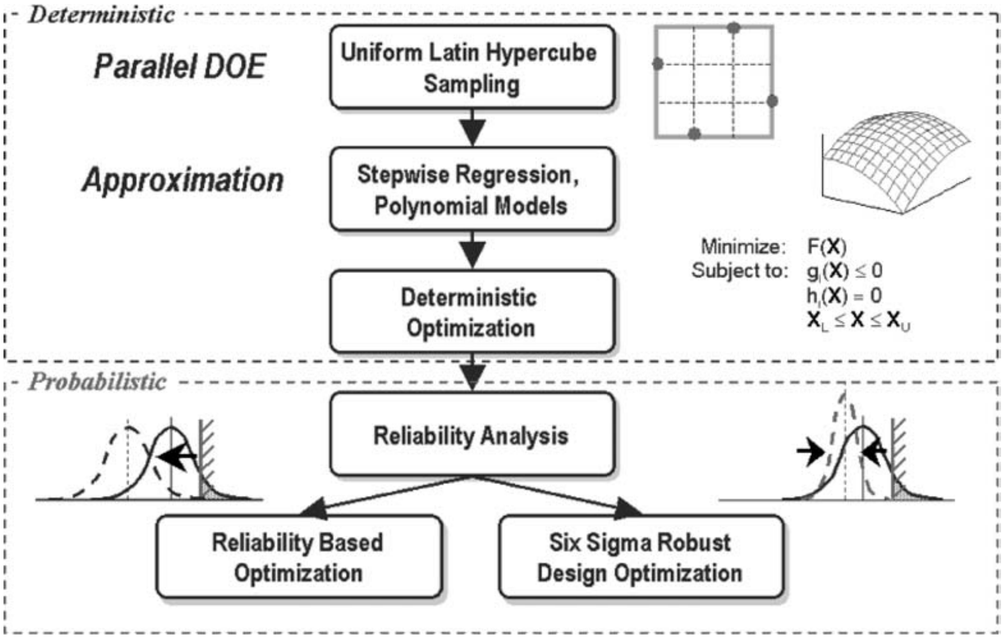


Fig. 5 Probabilistic analysis using approximation methods (Koch 2002)

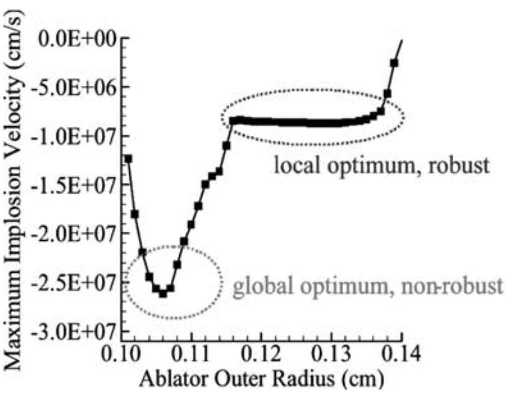


Fig. 6 Robust design in shock physics (Eldred *et al.* 2002b)

Giunta presented the following formulation for simulation-based optimization under uncertainty:

$$\begin{aligned} \text{minimize:}\quad & f(x)+W^T S(x,u) \\ \text{subject to:}\quad & g_L \le g(x) \le g_U \\ & a_L \le A^T S(x,u) \le a_U \\ & x_L \le x \le x_U \\ & x \in R^n \\ & u \text{ are probabilistic (Normal Weibull Etc)} \end{aligned} \tag{1}$$

where $S(x,u)$ are statistical metrics (e.g. means, standard deviations, failure probabilities, etc.) and W and A are weighting vectors/matrices. Approximation models are employed for $f(x)$, $g(x)$, and $S(x,u)$ to reduce the computational expense of these analyses. Detailed results for the computational shock physics example shown in Fig. 6 can be found in Eldred *et al.* (2002b). Giunta also mentioned that approximation models are useful for reducing the numerical noise that might occur in the output responses, citing his earlier work wherein response surface models helped smooth numerical noise in an aerodynamic analysis example (Giunta *et al.* 1994). While optimization and uncertainty quantification are becoming more important, they are still not viewed as critical path items at Sandia; he said the focus is still on "getting the physics right".

6 Challenge 4: Handling problems with large numbers of variables

Often referred to as the "curse of dimensionality" (Balabanov *et al.* 1996; Evans and Swartz 2000; Koch *et al.* 1999) a constant challenge in building accurate approximation models is handling problems with large numbers of variables: the more design variables you have, the more samples you need to build an accurate metamodel. This becomes increasingly important when modelling uncertainty because the design (input) variables and the uncertain (noise) variables must be captured in the model, thereby increasing the dimensionality of the design space even more.

Screening experiments are often employed to reduce the set of factors to those that are most important to the response(s) being investigated. Statistical experimentation is used to define the appropriate design analyses that must be run to evaluate the desired effects of the factors. Often two-level fractional factorial designs (Montgomery 1997) or Plackett–Burman (Plackett and Burman 1946) designs are used for screening, and only main (linear) effects of each factor are investigated.

Among the earliest such work, Box and Draper (1969) proposed a method to gradually refine a response surface model to better capture the real function by "screening" out unimportant variables. Ghosh discussed the use of intermediate design variables to reduce the dimensionality of the design space; a topology optimization example of an automobile body to improve structural rigidity was given as an example (Leiva *et al.* 2001). The variable-complexity response surface modelling method uses analyses of varying fidelity to reduce the design space to the region of interest (Balabanov *et al.* 1999; Giunta *et al.* 1996; Venter *et al.* 1998). A procedure for screening variables is offered by Welch *et al.* (1992) which uses a kriging-based approximation methodology to identify important variables, detect curvature and interactions, and produce a useful approximation model for two 20 variable problems using only 30–50 runs of the computer code. Booker noted, however, that the interaction between screening methods and optimization still needs to be investigated further. For instance, variables that might not be important during initial experimentation may become important in the later stages of the optimization such that the variables that were initially "screened out" need to be added back into the model.

Problems involving mixed discrete/continuous variables were also mentioned as one of the challenges facing the design of experiments for building approximation models. Booker emphasized that judicious selection of the experimental design is needed when factors with discrete levels are considered. For instance, the design variables for the power system examples (Karimi *et al.* 1996, 1997) mentioned in Sect. 2 had ON/OFF levels, mandating the use of an experimental design with two levels. Orthogonal arrays with discrete level choices are also available for problems with two or more discrete levels (Owen 1992). In general, problems with both continuous and discrete variables require special consideration and have thus far been solved largely on a problem-by-problem basis.

7
Closing remarks and future directions

The discussion that followed the presentations by the panelists revolved primarily around the research topics outlined in the previous sections. Two additional topics that continued to surface during the discussion involved using gradient information in approximation models and sequential methods for model fitting and building. Yang stated that gradient information was usually not readily available in their crashworthiness models; therefore, he did not advocate the use of gradient-enhanced approximations because obtaining gradient information added computational expense. Booker and Giunta agreed that if the information was readily available, or could be easily obtained through procedures such as automatic differentiation (Su and Renaud 1997), then it should be used to improve the accuracy of the approximation model; Booker recommended a paper by Morris *et al.* (1993) that offered a method for using gradient information in kriging models and a paper by Koehler (1997) that discusses the use of gradient information in kriging models and its usefulness for estimating transmitted variation. Methods for using gradient information to enhance approximation models were also being developed by several members of the audience (Liu and Batill 2000, 2002; van Keulen and Vervenne 2002).

Sequential and adaptive approximation methods were also being developed by several members of the audience (Pérez *et al.* 2002a,b,c; Rodríguez *et al.* 2001). A sequential method combining response surface models and kriging models was also mentioned (Wang and Simpson 2002), which used "inherited" sample points in Latin hypercube designs as new samples were taken (Wang 2003). The merits of sequentially sampling the design space (Farhang-Mehr and Azarm 2002) to improve the accuracy of the approximation model in one or more regions of interest were also discussed. The work by Osio and Amon (1996)was cited for their multi-stage sampling procedure for building kriging models.

Kriging models for approximation and global optimization were another big topic of discussion. In fact, more papers involving kriging-based approximation models appeared at the 2002 *MA&O Symposium* than at the past symposiums combined. Global optimization procedures using kriging models were discussed (Booker *et al.* 1999; Sasena *et al.* 2002; Audet *et al.* 2000), and a procedure for calibrating a kriging model during optimization that avoided problems with an ill-conditioned correlation matrix was discussed by Booker (2000b), see Fig. 7. Procedures for updating the theta parameters in a kriging model during continuous experimentation are investigated in Martin and Simpson (2002).

In addition to outlining research directions for advancing approximation methods themselves, panelists also charged the academic community with helping to educate engineers in how to use them. Ghosh emphasized that engineers should gain some basic exposure to approximation methods and their uses. He said that a strong theor-

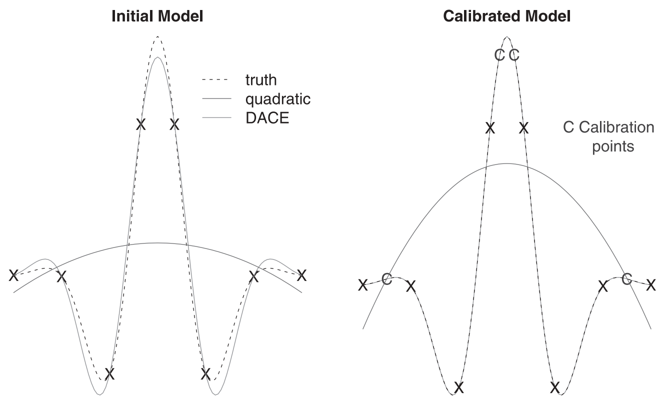


Fig. 7 Kriging model calibration during optimization (Booker 2000b)

etical background was not necessary, but it was important to know how to formulate a problem and interpret results to identify when problems occur. Koch echoed his comments, stating that a basic level of understanding is needed to build, validate, and exercise approximation models even though the majority of these processes are automated by software packages. A similar philosophy is used in academia when teaching finite element methods prior to using finite element software.

Giunta also stated that many engineers and analysts do not have sufficient background in applied mathematics (i.e. optimization) and statistics to understand approximation methods and how they are used. They are often unfamiliar with the statistical terms and concepts and are overwhelmed by the many choices available for the experimental design (e.g. central composite designs, Latin hypercubes, uniform designs, orthogonal arrays) and the approximation model (e.g. kriging, response surfaces, neural network, etc.). He closed in saying that good graphical user interfaces can help mitigate this but considerable "hand-holding" is needed in the meantime. Booker made similar comments, stating that it is helpful to know what an engineer plans to do with the results (e.g. identify main effects, screen variables, use the approximation for optimization) since that often dictates the approach and tools employed in the study.

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