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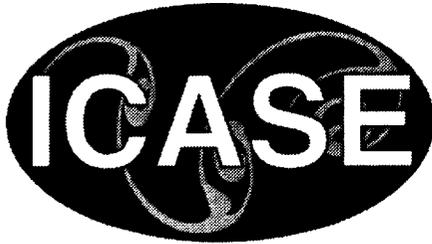
Comparison of Response Surface and Kriging Models in the Multidisciplinary Design of an Aerospike Nozzle

Timothy W. Simpson

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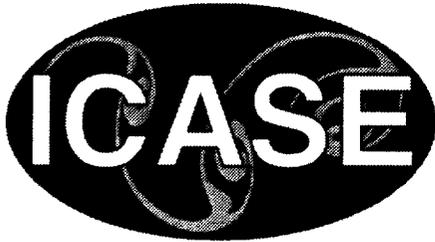
Comparison of Response Surface and Kriging Models in the Multidisciplinary Design of an Aerospike Nozzle

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COMPARISON OF RESPONSE SURFACE AND KRIGING MODELS IN THE MULTIDISCIPLINARY DESIGN OF AN AEROSPIKE NOZZLE

TIMOTHY W. SIMPSON[']

Abstract. The use of response surface models and kriging models are compared for approximating non-random, deterministic computer analyses. After discussing the traditional response surface approach for constructing polynomial models for approximation, kriging is presented as an alternative statistical-based approximation method for the design and analysis of computer experiments. Both approximation methods are applied to the multidisciplinary design and analysis of an aerospike nozzle which consists of a computational fluid dynamics model and a finite element analysis model. Error analysis of the response surface and kriging models is performed along with a graphical comparison of the approximations. Four optimization problems are formulated and solved using both approximation models. While neither approximation technique consistently outperforms the other in this example, the kriging models—using only a constant for the underlying global model and a Gaussian correlation function—perform as well as the second order polynomial response surface models.

Key words. response surface models, kriging, multidisciplinary design

Subject classification. Applied and Numerical Methods

1. Introduction. Current engineering analyses rely heavily on running complex, and often expensive, computer analysis codes. Despite the steady and continuing growth of computing power and speed, the complexity of these codes seems to keep pace with computing advances. Statistical techniques are widely used in engineering design to construct *approximations* of these analysis codes; these approximations are then used in lieu of the actual analysis codes, offering the following benefits.

- They yield insight into the relationship between (output) responses, **y**, and (input) design variables, **x**.
- They provide fast analysis tools for optimization and design space exploration since the cheap-to-run approximations replace the expensive-to-run computer analyses.
- They facilitate the integration of discipline dependent analysis codes.

The most common method for building approximations of computer analyses is to apply design of experiments (DOE), response surface (RS) models, and regression analysis to build second order polynomial approximations of the computationally expensive analyses. For example, the Robust Concept Exploration Method (see, e.g., [5] and [6]) has been developed to facilitate quick evaluation of different design alternatives, identify important design drivers, and generate robust top-level design specifications using DOE, RS models, and the compromise Decision Support Problem [25]; it has been successfully applied to the multiobjective design of a high speed civil transport (see, e.g., [5] and [19]), a family of General Aviation aircraft [40], a turbine lift engine [18], and a flywheel [22]. In other work, the Variable Complexity Response Surface Modeling (VCRSM) method (see, e.g., [12] and [13]) uses analyses of varying fidelity to reduce the design space to the region of interest and build response surface models of

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increasing accuracy. The VCRSM method employs DOE and RS modeling techniques and has been successfully applied to the multidisciplinary wing design of a high speed civil transport (see, e.g., [14] and [17]), to the analysis and design of composite curved channel frames [24], and to reduce numerical noise inherent in structural analyses (see, e.g., [14] and [45]) and shape design problems using fluid flow analysis [29]. A review of several applications of response surfaces in mechanical and aerospace engineering design is given in [41].

The use of response surfaces for approximating deterministic (i.e., non-random) computer analyses is statistically questionable due to the lack of random error in the computer model (cf., [41]). A more appropriate and perhaps more "statistically sound" method for approximating deterministic computer experiments is through the use of kriging [9] models which are also referred to as the Design and Analysis of Computer Experiments (DACE) models (see, e.g., [4], [20], and [38]). The validity of the kriging model is not dependent on the existence of random error and may therefore be better suited for applications involving deterministic computer experiments. Furthermore, kriging models interpolate between data points which may be yield more accurate results since computer experiments typically do not contain random error (i.e., you get the same output when you use the same input).

Booker [2] contrasts traditional DOE and RS modeling with DACE models. In the "classical" design and analysis of physical experiments, random variation is accounted for by spreading the sample points out in the design space and by taking multiple data points (replicates), see FIG. 1. Sacks, et al. [38] state that the [ ]classical notions of experimental blocking, replication, and randomization are irrelevant when it comes to deterministic computer experiments; thus, sample points should be chosen to fill the design space. They suggest minimizing the integrated mean squared error (IMSE) over the design region by using IMSE-optimal designs such as the one shown in the top right corner of FIG. 1.

	DOE/RS Modeling for Physical Experiments	DACE/Kriging for Computer Experiments
Experimental Design Input settings at which to obtain output	Account for Variability 	Space Filling
Models Inexpensive model to estimate output at untried input	Least Squares Fit 	Maximum Likelihood Estimate
Validation Determine fit accuracy	t-tests, F-statistics R^2, Residual plots [28]	Cross-validation Integrated mean square error [38]
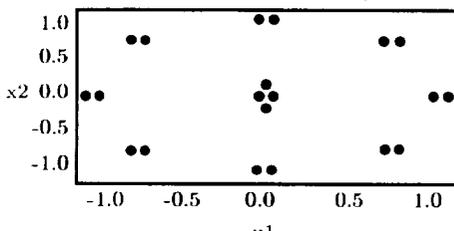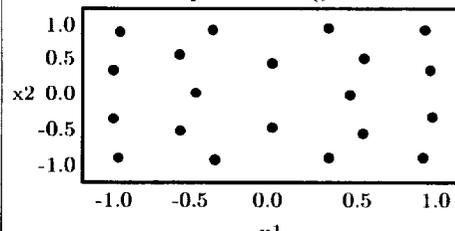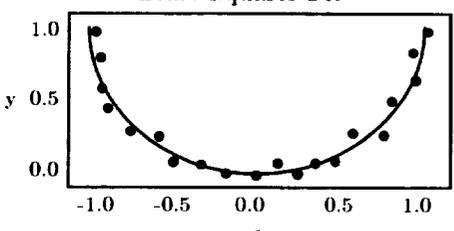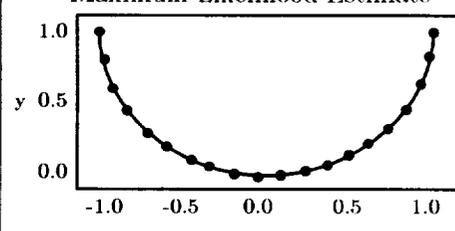
FIG. 1. ComparisonofDOE/RSmodelingandDACE/Kriging(adaptedfrom[2]).

As shown in the middle of FIG. 1, response surface modeling typically employs least squares regression to fit a polynomial model to the sampled data; kriging models are chosen to interpolate the data and are fit using maximum likelihood estimation (see, e.g., [20]). Validation of RS models is 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 (see, e.g., [28]). Sacks, et al. [38] and Welch, et al. [47] both state that statistical testing is inappropriate when it comes to deterministic computer experiments which lack random error; cross-validation and integrate mean square error can be utilized to assess the accuracy of a kriging model.

DACE and kriging models have found limited application in engineering design perhaps because of the lack of readily available software to fit kriging models, the added complexity of fitting a kriging model, or the additional effort required to use a kriging model. To clarify this last point, prediction with a kriging model requires the inversion and multiplication of several matrices, and the kriging model does not exist as a "closed-form" polynomial equation. RS model prediction only requires computation of simple polynomial equation once a model has been fit. The goal in this paper is to examine the added computational expense required to perform kriging and compare the predictive capability of kriging and RS models.

In Section 2 an overview of the statistical and mathematical foundations of response surface modeling and kriging is given. In Section 3 the multidisciplinary design of an aerospike nozzle is introduced; it serves as a test problem to compare RS and kriging models for approximation. In Section 4 the RS and kriging models are constructed for the aerospike nozzle example. In Section 5 four optimization problems are formulated and solved using the RS and kriging models; Section 6 contains a discussion of ongoing work.

2. Statistical Approximations for Computer Experiments. Building approximations of computer analyses typically involves: (a) choosing an experimental design to sample the computer analysis code, (b) choosing a model to represent the data, and (c) fitting the model to the observed data. There are a variety of options for each of these steps as shown in FIG. 2, and some of the more prevalent ones have been highlighted.

EXPERIMENTAL DESIGN	MODEL CHOICE	MODEL FITTING	SAMPLE APPROXIMATION TECHNIQUES
(Fractional) Factorial	Polynomial (linear, quadratic)	Least Squares Regression	Response Surface Methodology
Central Composite	Splines (linear, cubic)	Weighted Least Squares Regression	
Box-Behnken			
D-Optimal	Realization of a Stochastic Process	Best Linear Unbiased Predictor	Kriging
Orthogonal Array			
Plackett-Burman	Kernel Smoothing	Best Linear Predictor	
Hexagon	Radial Basis Functions		Neural Networks
Hybrid		Backpropagation	
Latin Hypercube	Network of Neurons	Log-Likelihood	
Select By Hand			
Random Selection	Rulebase or Decision Tree	Entropy (info.-theoretic)	Inductive Learning

FIG. 2. *Techniques for building approximations* [41].

Simpson, et al. [41] discuss several of the advantages and disadvantages of the highlighted approaches listed in FIG. 2, namely, response surface methodology, neural networks, inductive learning and kriging. In this work, the model choice and model fitting portions of building approximations are the primary concern; response surface models are discussed in Section 2.1 and kriging models in Section 2.2. It is assumed that the reader has some knowledge of DOE and RS modeling and little to no knowledge of kriging.

2.1. Overview of Response Surface Modeling. Response surface modeling techniques were originally developed to analyze the results of physical experiments and create empirically-based models of the observed response values. Response surface modeling postulates a model of the form:

$$(1) \qquad y(\mathbf{x}) = f(\mathbf{x}) + \varepsilon$$

where $y(\mathbf{x})$ is the unknown function of interest, $f(\mathbf{x})$ is a known polynomial function of $\mathbf{x}$, and ε is random error which is assumed to be normally distributed with mean zero and variance σ^2. The individual errors, ε_i, at each observation are also assumed to be independent and identically distributed. The polynomial function, $f(\mathbf{x})$, used to approximate $y(\mathbf{x})$ is typically a low order polynomial which is assumed to be either linear as given by EQN. (2):

$$(2) \qquad \hat{y} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i$$

or quadratic as given by EQN. (3):

$$(3) \qquad \hat{y} = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{ii=1}^{k} \beta_i x_{ii}^2 + \sum \sum_{i<j} \beta_{ij} x_i x_j$$

The parameters β_0, β_i, β_{ii}, and β_{ij}, of the polynomials in EQNS. (2) and (3) are determined through least squares regression which minimizes the sum of the squares of the deviations of the predicted values, $\hat{y}(x)$, from the actual values, $y(x)$. In order to fit the model to the observed data using least squares regression, the coefficients of EQNS. (2) and (3) can be estimated using EQN. (4).

$$(4) \qquad\qquad \beta=[X'X]^{-1}X'y$$

In EQN. (4), X is the design matrix of sampled points, and y is a column vector containing the corresponding values of the response. For more details on least squares regression or polynomial RS modeling see, e.g., [28].

2.2. Overview of Kriging.

2.2.1. Mathematics of Kriging.
Kriging, or DACE modeling, postulates a combination of a polynomial model plus departures of the form given by EQN. (5):

$$(5) \qquad\qquad y(x) = f(x) + Z(x)$$

where $y(x)$ is the unknown function of interest, $f(x)$ is a known polynomial function of x, and $Z(x)$ is the realization of a normally distributed Gaussian random process with mean zero, variance σ^2, and non-zero covariance. The $f(x)$ term in EQN. (5) is similar to the polynomial model in a response surface and provides a "global" model of the design space; in many cases $f(x)$ is simply taken to be a constant term β (see, e.g., [20], [38], and [47]).

While $f(x)$ "globally" approximates the design space, $Z(x)$ creates "localized" deviations so that the kriging model interpolates the n_s sampled data points. The covariance matrix of $Z(x)$ is given by EQN. (6).

$$(6) \qquad\qquad \mathrm{Cov}[Z(x^i),Z(x^j)] = \sigma^2\, R([R(x^i,x^j)])$$

In EQN. (6), R is the correlation matrix, and $R(x^i,x^j)$ is the spatial correlation function between any two of the n_s sample points x^i and x^j. R is a $n_s \times n_s$ symmetric, positive definite matrix with ones along the diagonal. The correlation function $R(x^i,x^j)$ is specified by the user; Sacks, et al. [38] and Koehler and Owen [20] discuss several correlation functions. The Gaussian correlation function in EQN. (7) is employed in this work.

$$(7) \qquad\qquad R(x^i,x^j) = \exp(-\sum_{k=1}^{n_{dv}}\theta_k\left|x_k^i - x_k^j\right|^2)$$

The θ_k in EQN. (7) are the unknown parameters used to fit the model, n_{dv} is the number of design variables, and x_k^i and x_k^j are the kth components of sample points x^i and x^j. In some cases, using a single correlation parameter gives sufficiently good results (see, e.g., [4], [30], and [38]).

Predicted estimates, $\hat{y}(x)$, of the response $y(x)$ at untried values of x are given by EQN. (8):

$$(8) \qquad\qquad \hat{y}=\hat{\beta} +r^T(x)R^{-1}(y\text{-}F\hat{\beta})$$

where **y** is the column vector of length n_s which contains the values of the response at each sample point, and **F** is a column vector of length n_s which is filled with ones when f(**x**) is taken as a constant. In EQN. (8), **r**(**x**) is the correlation vector of length n_s between an untried **x** and the sampled data points [$\mathbf{x}^1$, $\mathbf{x}^2$, ..., $\mathbf{x}^{n_s}$] and is given by EQN. (9).

(9)
$$\mathbf{r}^T(\mathbf{x}) = [R(\mathbf{x},\mathbf{x}^1), R(\mathbf{x},\mathbf{x}^2), ..., R(\mathbf{x},\mathbf{x}^{n_s})]^T$$

In EQN. (8), $\hat{\beta}$ is estimated using EQN. (10).

(10)
$$\hat{\beta} = (\mathbf{F}^T\mathbf{R}^{-1}\mathbf{F})\mathbf{F}^T\mathbf{R}^{-1}\mathbf{y}$$

The estimate of the variance, $\hat{\sigma}^2$, of the sample points from the underlying global model (not the variance in the observed data itself) is given by EQN. (11):

(11)
$$\hat{\sigma}^2 = \frac{(\mathbf{y} - \mathbf{F}\hat{\beta})^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{F}\hat{\beta})}{n_s}$$

where f(**x**) is assumed to be the constant $\hat{\beta}$. The maximum likelihood estimates (i.e., "best guesses") for the θ_k in EQN. (7) used to fit the model are found by maximizing EQN. (12) over $\theta_k > 0$ (see, e.g., [4]).

(12)
$$\max_{\theta_k > 0} -\frac{[n_s \ln(\hat{\sigma}^2) + \ln(\det\mathbf{R})]}{2}$$

Both $\hat{\sigma}^2$ and $\det\mathbf{R}$ are functions of θ_k. While any values for θ_k create an interpolative model, the "best" kriging model is found by solving the k-dimensional unconstrained, non-linear, optimization problem given by EQN. (12).

2.2.2. Applications of DACE and Kriging.

DACE and kriging models have found limited use in engineering design applications since its introduction into the literature by Sacks, et al. [38]. Giunta [11] has performed a preliminary investigation into the use of DACE modeling for the multidisciplinary design optimization of a High Speed Civil Transport aircraft. He explores a 5 and a 10 variable design problem, observing that the DACE and response surface modeling approaches yield similar results due to the quadratic trend of the responses. Osio and Amon [30] have developed an extension of DACE modeling for numerical optimization which uses a multistage strategy for refining the accuracy of the model; they have applied their approach to the thermal design of an embedded electronic package which has 5 design variables. Welch, et al. [46] describe a kriging-based approximation methodology which they use 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; they claim their method can cope with up to 30-40 variables provided factor sparsity can be exploited. Booker, et al. [3] solve a 31 variable helicopter rotor structural design problem using an approximation method based on kriging. Booker [2] extends the helicopter rotor design problem to include 56 structural variables to examine the aeroelastic and dynamic response of the rotor. Trosset and Torczon [44] have developed a numerical optimization strategy which incorporates DACE modeling and pattern search methods for global optimization. Cox and John [7] have developed the Sequential Design for Optimization method which

uses lower confidence bounds on predicted values of the response for the sequential selection of evaluation points during optimization. Both approaches have shown improvements over traditional optimization approaches when applied to a variety of standard mathematical test problems.

2.3. One Variable Example of Response Surface and Kriging Models.

A simple one variable example bests illustrates the difference between the approximation capabilities of a second order RS model and a kriging model. Su and Renaud [42] formulated this example to demonstrate some of the limitations of using second order RS models; see FIG. 3. They fit a second order response surface using least squares regression to five sample points from a fabricated eighth order function within the region of the optimum (x = 932). A kriging model using a constant for the global model and the Gaussian correlation function of EQN. (7) is fit to the same five points; the original function, the five sample points, and the RS and kriging models are shown in FIG. 3.

Immediately evident from FIG. 3 is fact that the kriging model interpolates the data points, approximating the original function better than the response surface model and predicting an optimum which is much closer to the actual optimum. It is important to notice that outside of the design space defined by the sample points (920 < x < 945), neither model predicts well as expected; the kriging model returns to the underlying global model which is a constant. This is typical behavior for a kriging model; far from the sample points, the kriging model returns to the underlying global model since the influence of the sample points has exponentially decayed away outside of the design space.
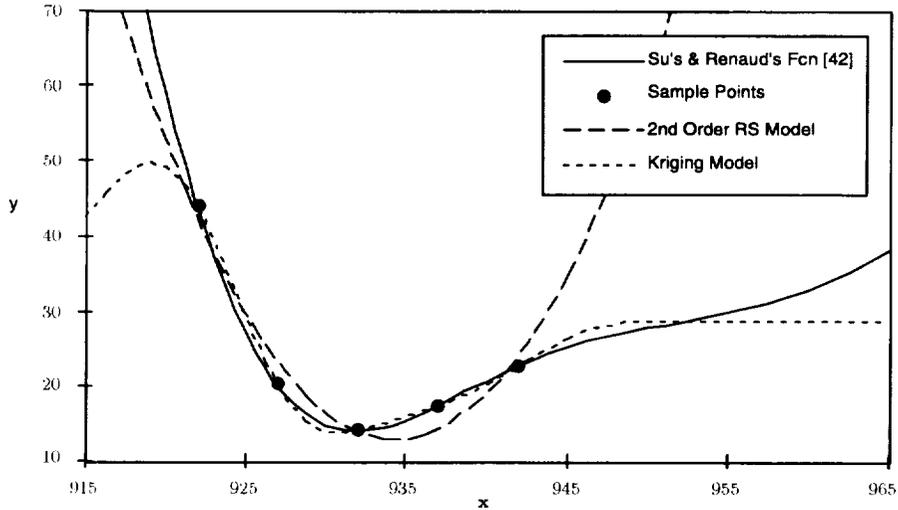
FIG. 3. *One variable example of response surface and kriging models.*

Sixteen evenly spaced points (not including the sample points) are taken from within the range (920 < x < 945) to check the accuracy of the two approximation models. The maximum absolute error (difference between the actual and predicted values), the average absolute error, and the root mean square error (MSE), which is:

$$(13) \qquad \text{root MSE} = \sqrt{\frac{\sum_{i=1}^{n_{error}} (y_i - \hat{y}_i)^2}{n_{error}}}$$

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where n_{error} is the number of points (= 16), are listed in TABLE 1. Based on the error analysis in TABLE 1, it can be concluded that the kriging model approximates the original function better since it has a lower root MSE, average error, and maximum error. A more involved multidisciplinary design example is described in the next section.

TABLE 1. *Error analysis for one variable example.*

	2nd Order RS Model	Kriging Model
Max ABS(error)	3.134	2.507
Avg ABS(error)	1.911	0.776
root MSE	2.155	1.004

3. Aerospike Nozzle Design Example. The multidisciplinary design of an aerospike nozzle has been selected as the test problem for comparing the predictive capability of RS and kriging models. The linear aerospike rocket engine is the propulsion system proposed for the VentureStar [43] reusable launch vehicle illustrated in FIG. 4.
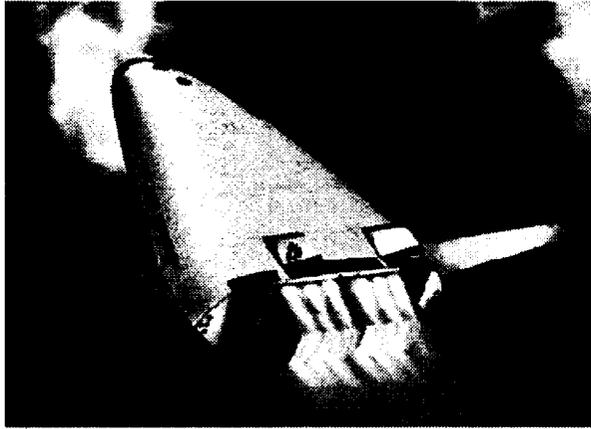
FIG. 4. *VentureStar reusable launch vehicle with linear aerospike propulsion system* [21].

The aerospike rocket engine consists of a rocket thruster, cowl, aerospike nozzle, and plug base regions as shown in FIG. 5. The aerospike nozzle is a truncated spike or plug nozzle that adjusts to the ambient pressure and integrates well with launch vehicles [34]. The flow field structure changes dramatically from low altitude to high altitude on the spike surface and in the base flow region (cf., [15], [27], and [36]). Additional flow is injected in the base region to create an aerodynamic spike [16] which gives the aerospike nozzle its name and increases the base pressure and contribution of the base region to the aerospike thrust.
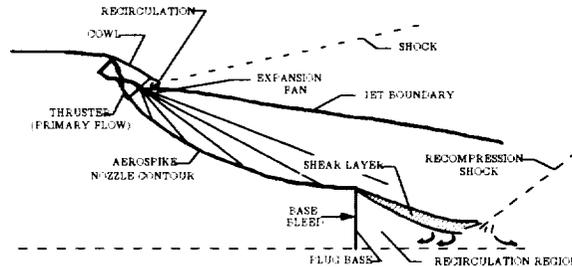
FIG. 5. *Aerospikecomponentsandflowfieldcharacteristics[21].*

The analysis of the nozzle involves two disciplines—aerodynamics and structures—since there is an interaction between the structural displacements of the nozzle surface and the pressures caused by the varying aerodynamic effects. Thrust and nozzle wall pressure calculations are made using computational fluid dynamics (CFD) analysis and are linked to a structural finite element analysis model for determining nozzle weight and structural integrity. A mission average engine specific impulse and engine thrust/weight ratio are calculated and used to estimate vehicle gross-lift-off-weight (GLOW) based on data supplied by Rocketdyne. The multidisciplinary domain decomposition is illustrated in FIG. 6. Korte, et al. [21] provide additional details on the aerodynamic and structural analyses for the aerospike nozzle.
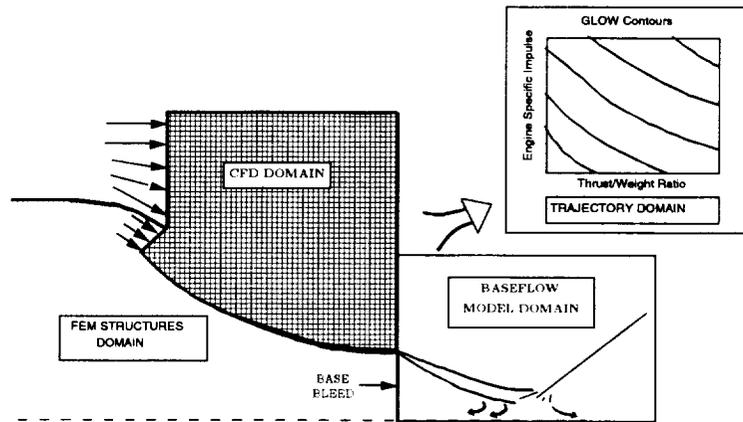
FIG. 6. *Multidisciplinarydomaindecomposition[21].*

For this study, three design variables are considered for the multidisciplinary design of the aerospike nozzle: thruster angle, base height, and length as shown in FIG. 7. The thruster angle is the entrance angle of the gas from the combustion chamber onto the nozzle surface; the base height and length refer to the solid portion of the nozzle itself. A quadratic model is created to generate values of spline knot surface angle slope and exit angle which define the nozzle profile, corresponding to specific values of thruster angle, base height, and length.
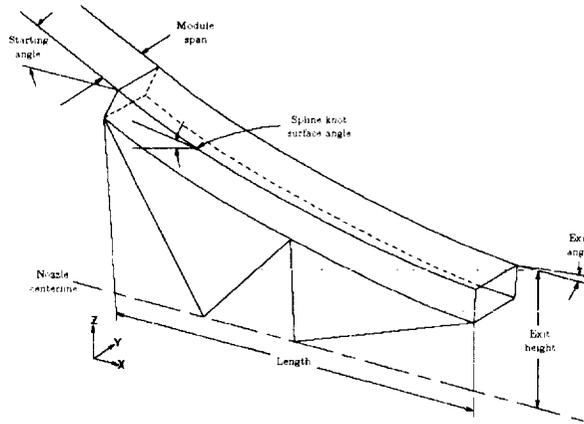
FIG. 7. *Nozzlegeometrydesignvariables[21].*

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Bounds for the design variables are set based on information from Boeing Rocketdyne and viable nozzle profiles from the quadratic model based on all combinations of thruster angle, height, and length within the design space. Second order RS models and kriging models are developed for each response—thrust, weight, and GLOW—in the next section; optimization of the aerospike nozzle using the RS and kriging models for different objective functions is performed in Section 5.

4. Approximations for the Aerospike Nozzle Problem. The data used to fit the RS and kriging models is obtained from a 25 point orthogonal array (bose 5 3 1 oarand) from [33]. The sample points are illustrated in FIG. 8 and are scaled to fit the three dimensional design space defined by the bounds on the thruster angle, base height, and length.
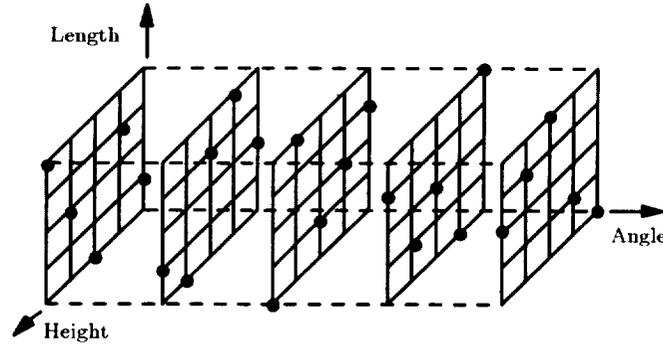
FIG. 8. Samplepointsforthogonalarray.

Section 4.1 contains the response surface models which are fit to the data; Section 4.2 contains the kriging models. Error analysis of the response surface and kriging models is discussed in Section 4.3, and a graphical comparison of the approximation models is given in Section 4.4.

4.1. Response Surface Models. The RS models for weight, thrust, and GLOW are obtained using ordinary least squares regression techniques and JMP [39]. The corresponding RS models are given in EQNS. (14)-(16). The equations have been scaled against the baseline design due to the proprietary nature of some of the data.

$$\text{Weight} = 0.810 - 0.116*a + 0.121*h + 0.152*l + 0.065*a^2 - 0.025*a*h +$$
$$0.0013*h^2 - 0.0539*a*l - 0.0131*h*l + 0.0301*l^2$$
(14)

$$\text{Thrust} = 0.9968 + 0.00031*a + 0.0019*h + 0.0060*l - 0.00175*a^2 + 0.00125*a*h -$$
$$0.0011*h^2 + 0.00125*a*l - 0.00198*h*l - 0.00165*l^2$$
(15)

$$\text{GLOW} = 0.9930 - 0.0270*a + 0.0065*h - 0.0265*l + 0.0307*a^2 - 0.0163*a*h +$$
$$0.0100*h^2 - 0.0226*a*l + 0.0151*h*l + 0.0195*l^2$$
(16)

The R^2, R^2-adjusted, and root MSE values for each of these second order RS models are summarized in TABLE 2. As evidenced by the high R^2 and R^2-adjusted and low root MSE values, the second order polynomial model appears to capture a large portion of the observed variance.

TABLE 2. *Modeldiagnosticsofresponsesurfacemodels.*

Measure	Response		
	Weight	**Thrust**	**GLOW**
R^2	0.986	0.998	0.971
R^2-adjusted	0.977	0.996	0.953
root MSE	1.12%	0.01%	0.25%

4.2. Kriging Models for the Aerospike Nozzle Problem.

The kriging models are built from the same 25 sample points used to fit the response surface models in Section 4.1. A constant term (i.e., the mean of the data) is selected for the underlying global model, and the Gaussian correlation function, EQN. (7), is utilized for the local departures determined by the correlation matrix **R**.

Initial investigations revealed that a single θ parameter was insufficient to accurately model the data due to scaling of the design variables. Therefore, a simple 3-D exhaustive grid search with a refinable step size was used to find the maximum likelihood estimates for the three θ parameters needed to obtain the "best" kriging model. The resulting maximum likelihood estimates for the three θ parameters for the weight, thrust, and GLOW models are summarized in TABLE 3; these values are for the scaled sample points.

TABLE 3. *Thetaparametersforkrigingmodels.*

	Response		
	Weight	**Thrust**	**GLOW**
$\theta_{angle} =$	0.5481	0.30	3.362
$\theta_{height} =$	1.323	0.50	2.437
$\theta_{length} =$	2.718	0.65	0.537

With these parameters and the corresponding 25 sample points, the kriging models are fully specified. A new point is predicted using these θ values in combination with EQNS. (8)-(10). The accuracy of the RS and kriging models is examined in the next two sections.

4.3. Error Analysis of Response Surface and Kriging Models.

An additional 25 randomly selected points are used to verify the accuracy of the RS and kriging models. Error is defined as the difference between the actual response from the computer analysis, y(**x**), and the predicted value, $\hat{y}$ (**x**), from the RS or kriging model. The maximum absolute error, the average absolute error, and the root MSE, EQN. (13), for the 25 randomly selected points are summarized in TABLE 4.

TABLE 4. *Erroranalysisofapproximationmodels.*

SecondOrderResponseSurfaceModels

	Weight	Thrust	GLOW
Max ABS(error)	19.57%	0.032%	3.68%
Avg ABS(error)	2.44%	0.012%	0.53%
root MSE	4.54%	0.015%	0.90%

KrigingModels(withconstantterm)

	Weight	Thrust	GLOW
Max ABS(error)	17.23%	0.048%	3.43%
Avg ABS(error)	2.51%	0.012%	0.59%
root MSE	4.37%	0.018%	0.89%

For the weight and GLOW responses, the kriging models have lower maximum absolute errors and lower root MSEs than the RS models; however, the average absolute error is slightly larger for the kriging models indicating that the average magnitude of the prediction error is larger for the kriging models than the RS models. As for thrust, the RS models are slightly better than the kriging models according to the values in the table; the maximum absolute error and root MSE are slightly less while the average absolute errors are essentially the same. It is not surprising that the RS model predicts thrust better; it has a very high R^2 value, 0.998, and low root MSE, 0.01%. It is reassuring to note, however, that the kriging model, despite using a constant term for the underlying global model, is only slightly less accurate than the corresponding RS model. It appears that both approximations predict reasonably well with the kriging models having a slight overall advantage because of the lower root MSE values.

4.4. Graphical Comparison of Response Surface and Kriging Models. In addition to the error analysis of Section 4.3. a graphical comparison of the RS and kriging models has been performed to visualize differences in the two approximation models. In FIGS. 9-11, 3-D contour plots of thrust, weight, and GLOW as a function of angle, length, and base height are given. In each figure, the same contour levels are used for the RS and kriging models so that the shapes of the contours can be compared.
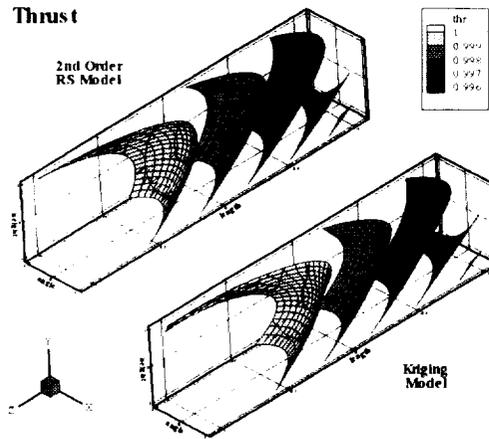
FIG. 9. *Response surface and kriging models for thrust.*

In FIG. 9, it can be seen that the contours of thrust for the RS and kriging models are very similar. As evidenced by the high R^2 and low root MSE values, the RS model fits the data quite well, and it is reassuring to note that the kriging model resembles the RS model even through the underlying global model for the kriging model is just a constant term.
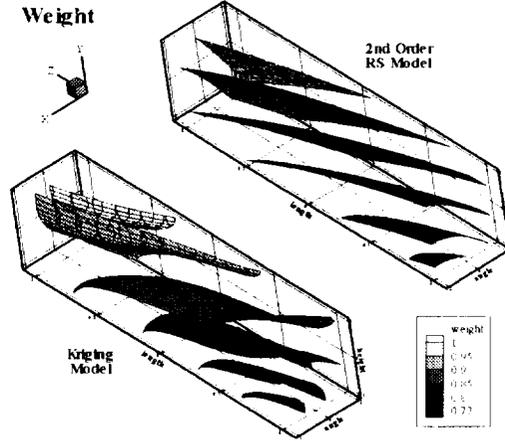
FIG. 10. *Responsesurfaceandkrigingmodelsforweight.*

The contours of the RS and kriging models for weight in FIG. 10 are also very similar, but the influence of the localized perturbations caused by the Gaussian correlation function in the kriging model can begin to be seen. The error analysis from Section 4.3 indicated that the kriging model for weight is slightly more accurate than the RS model which may result from the small localized variations.

A. *Isometricview.*   B. *Endview.*
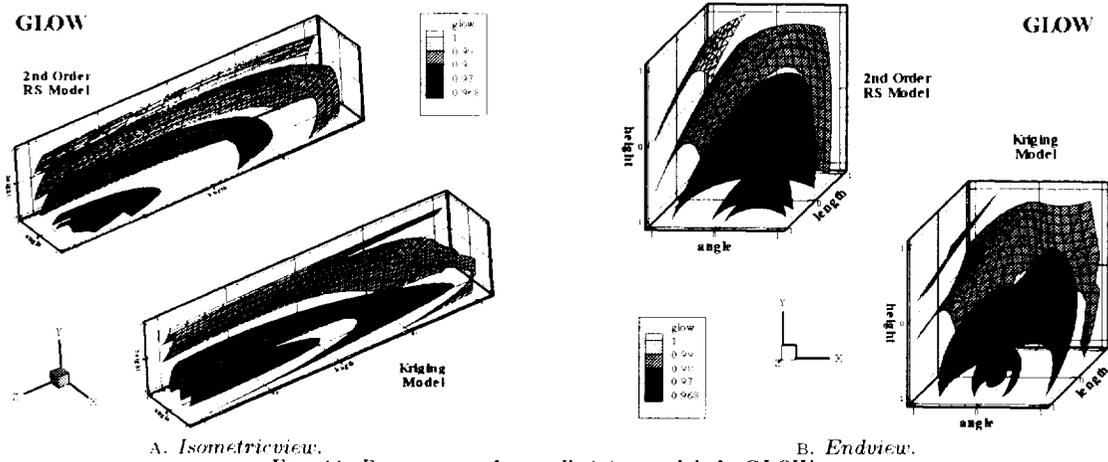
FIG. 11. *ResponsesurfaceandkrigingmodelsforGLOW.*

The general shape of the GLOW contours is the same in FIG. 11A, however, the size and shape of the different contours, particularly along the length axis, are quite different. The end view along the length axis in FIG. 11B further highlights the differences between the two models. Notice also in FIG. 11B that the kriging model predicts a minimum GLOW within the design space centered around Height=-0.8, Angle=0, along the axis defined by 0.2 < Length < 0.8; this minimum was verified through additional experiments.

5. Optimization Using Response Surface and Kriging Models. The true test of the accuracy of the RS and kriging models comes when the approximations are used in optimization. It is crucial that any approximations used in optimization prove reasonably accurate, lest they lead the optimization algorithm into regions of bad designs. Trust Region approaches (see, e.g., [23] and [35]) and the Model Management framework (see, e.g., [4] and [10]) have been developed to ensure that optimization

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algorithms are not led astray by inaccurate approximations. In this work, however, the focus has been on developing the approximation models, particularly the kriging models, and not on the optimization itself.

Four different optimization problems are formulated and solved to compare the accuracy of the RS and kriging models: (1) maximize thrust, (2) minimize weight, (3) minimize GLOW, and (4) maximize thrust/weight ratio. The first two objective functions represent traditional single objective, single discipline optimization problems. The second two objective functions are more characteristic of multidisciplinary optimization; minimizing GLOW or maximizing the thrust/weight ratio requires trade-offs between the aerodynamics and structures disciplines. For each objective function, constraint limits are placed on the remaining responses; for instance, constraints are placed on the maximum allowable weight and GLOW and the minimum allowable thrust/weight ratio when maximizing thrust. However, none of the constraints are active or binding in any of the final results.

Each optimization problem is solved using: (a) the RS model approximations and (b) the kriging model approximations for thrust, weight, and GLOW. The optimization is performed using a Generalized Reduced Gradient (GRG) algorithm. Three different starting points are used for each objective function (the lower, middle, and upper bounds of the design variables) to assess the average number of analysis and gradient calls necessary to obtain the optimum design within the given design space; the solutions for each objective for each approximation converge to the same optimum despite the initial starting point. The same parameters (i.e., step size, tolerance, constraint violation, etc.) are used within the GRG algorithm for each optimization. The optimization results are summarized in TABLE 5. Design variable and response values have been scaled as a percentage of the baseline design due to the proprietary nature of some of the data.

TABLE 5. *Optimizationresultsusingresponsesurfaceandkrigingmodels.*

	Avg. # of Analysis Calls	Avg. # of Gradient Calls	Optimum Design		Predicted Optimum		Verified Optimum	% Error*
Maximize Thrust								
RS Models	27	4	Angle	0.096	Thrust	1.0016	1.0013	0.02%
			Height	-0.433	Weight	0.9450	0.9476	-0.27%
			Length	1.000	Thr/Wt	1.0141	1.0134	0.07%
					GLOW	0.9724	0.9759	-0.36%
Kriging Models	62	5	Angle	0.656	Thrust	1.0016	1.0014	0.02%
			Height	-0.627	Weight	0.9385	0.9155	2.51%
			Length	1.000	Thr/Wt	1.0157	1.0210	-0.51%
					GLOW	0.9690	0.9683	0.08%
Minimize Weight								
RS Models	29	3	Angle	0.800	Thrust	0.9957	0.9957	-0.01%
			Height	-1.000	Weight	0.7584	0.7496	1.18%
			Length	-1.000	Thr/Wt	1.0533	1.0555	-0.21%
					GLOW	0.9936	0.9906	0.30%
Kriging Models	43	4.67	Angle	1.000	Thrust	0.9965	0.9956	0.08%
			Height	-0.873	Weight	0.7725	0.7443	3.79%
			Length	-1.000	Thr/Wt	1.0506	1.0568	-0.59%
					GLOW	0.9824	0.9914	-0.90%
Minimize GLOW								
RS Models	30.67	3.33	Angle	0.616	Thrust	1.0013	0.9957	0.56%
			Height	-1.000	Weight	0.8969	0.8617	4.09%
			Length	1.000	Thr/Wt	1.0251	1.0286	-0.34%
					GLOW	0.9660	1.0146	-4.79%
Kriging Models	57.67	6.33	Angle	0.764	Thrust	1.0009	1.0006	0.04%
			Height	-0.833	Weight	0.9060	0.8732	3.75%
			Length	0.676	Thr/Wt	1.0228	1.0302	-0.72%
					GLOW	0.9675	0.9680	-0.05%
Maximize Thrust/Weight Ratio								
RS	27	4	Angle	0.096	Thrust	1.0016	0.9959	0.57%
			Height	-0.433	Weight	0.9450	0.9073	4.16%

Models			Length	1.000	Thr/Wt	1.0141	1.0173	-0.31%
					GLOW	0.9724	1.0228	-4.93%
Kriging *Models*	62	5	Angle	0.656	Thrust	1.0016	1.0014	0.02%
			Height	-0.627	Weight	0.9385	0.9063	3.56%
			Length	1.000	Thr/Wt	1.0157	1.0231	-0.73%
					GLOW	0.9690	0.9666	0.25%

*$A(+)$ error term indicates that the model is overpredicting, $a(-)$ indicates that it is underpredicting.

The following observations can be made based on the data in TABLE 5.

- *Average number of analysis and gradient calls:* In general, the RS models require fewer analysis and gradient calls to achieve the optimum than the kriging models do. This can be attributed to the fact that the RS models are simple second order polynomials whereas the kriging models are more complex.

- *Convergence rates:* Although not shown in the table, optimization using the RS models tends to converge more quickly than when using kriging models. This can be inferred from the average number of gradient calls which is one to three calls fewer for the RS models.

- *Optimum designs:* The optimum designs obtained from the RS and kriging models are essentially the same for each objective function, indicating that both approximations send the optimization algorithm in the same general direction. The largest discrepancy is the length for the minimize GLOW optimization; RS models predict the optimum GLOW occurs at the upper bound on length (+1) while the kriging models yield 0.676. This difference is evident in FIG. 11.

- *Predicted optima and prediction errors:* To check the accuracy of the predicted optima, the optimum design values for angle, height, and length are used as inputs into the original analysis codes and the percentage difference between the actual and predicted values is computed. The prediction error is less than 5% for all cases and is 0.5% or less in three quarters of the results.

In summary, then, neither model consistently outperforms the other, and the difference in predictive capability of each model for each objective function is quite small. *The kriging models perform as well as the second order RS models even though the global portion of the kriging model is only a constant.* Ongoing work to improve model accuracy and checking adequacy of fit is detailed in the next section.

6. Closing Remarks and Future Work. This work represents a preliminary investigation into the use of kriging as an alternative statistical-based approximation technique for modeling non-random, deterministic computer experiments. A three variable engineering design example is used to compare the approximation capability of response surface modeling and kriging. The example is the multidisciplinary design of an aerospike nozzle which includes a CFD and a finite element model. With this simple, yet realistic engineering example, the use of kriging models as an alternative approximation technique has been demonstrated. At this point, there is inconclusive evidence to state that one approximation method is more advantageous than another; however, the kriging models, using only a constant underlying global model and a Gaussian correlation function, perform as well as the second order response surface models.

There are several research issues to address for the application of kriging and DACE methods for other (and larger) engineering design problems.

- *Fitting a kriging model:* Fitting a kriging model requires solution of an k-dimensional, unconstrained, non-linear optimization problem, EQN. (12), in order to determine the maximum likelihood estimates of the θ parameters for the "best" kriging model. Pattern search methods and simulated annealing algorithms are currently being employed to perform this optimization. For small problems with relatively few sample points, this optimization is rather trivial. However, as the size of the problem

increases and the number of sample points increases, the added effort needed to obtain the "best" kriging model may quickly begin to outweigh the benefit of building the approximation.

- *Selecting a kriging model:* In this example, a constant is used for the global portion of the kriging model based on the success of the work in [30], [37], and [47]. However, using a global polynomial model for f(x) in Eqn. (5) may further improve the accuracy of the kriging model. Giunta [11] performs a preliminary investigation of such an approach and finds that minimal improvement was obtained.

- *Predicting with a kriging model:* Unlike RS model prediction, prediction with a kriging model requires the inversion and multiplication of several matrices; these matrices grow as the number of sample points increases. For large problems, prediction with the kriging model may become computationally expensive in and of itself. Furthermore, it is more difficult to look at a kriging model and determine the effects of the design variables on the response(s) since the global model is usually taken as a constant, and each prediction point is essentially the sum of exponentially decaying functions based on **R**.

- *Validating a kriging model:* With RS models, R^2 values and residual plots can be used to assess model fit and accuracy. Since kriging models interpolate the data, there are no residuals and alternative checks must be implemented to validate the model. In this example an additional 25 random data points are used to check model adequacy; however, more formal approaches exist. Otto, et al. [31] and [32] and Yesilyurt and Patera [48] have developed a Bayesian-validated surrogate approach which uses additional validation points to make qualitative assessments of the quality of the approximation model and provide theoretical bounds on the largest discrepancy between the model and the actual computer analysis. An alternative method which does not require additional points is leave-one-out cross validation [26]. Each sample point used to fit the model is removed one at a time, the model is rebuilt without the sample point, and the difference between the model without the sample point and actual value at the sample point is computed for all of the sample points. Neither approach was implemented in this example due to the increased computation effort required.

- *Design of experiments for building kriging models:* Are there designs which are better suited for sampling computer experiments and building kriging models than for sampling physical experiments and building RS models? The opinions on the appropriate experimental design vary; the only consensus reached thus far is that designs for non-random, deterministic computer analyses should be space filling. In this example, orthogonal arrays are used to build approximation following the work by Booker, et al. [3] and [4]. Giunta [11] uses D-optimal designs to fit his kriging and RS models; Sacks, et al. [38] suggest using IMSE-optimal designs; and Koehler and Owen [20] discuss minimax, maximin, Latin hypercube, and scrambled net designs for computer experiments.

Despite the added complexity of fitting, using, and validating a kriging model, the potential gains in model accuracy justify continued investigation into the approach. The kriging software under development will facilitate the use and validation of kriging models, increasing their attractiveness for engineering applications. Finally, future work on the aerospike nozzle design problem includes expanding the scope of the problem to include more design variables and responses and investigating the impact of decomposing the problem into its disciplines by building approximation models of each discipline separately and examining the effect of different multidisciplinary design formulations (e.g., [1] and [8]) on the solution.

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