

Kriging Models for Global Approximation in Simulation-Based Multidisciplinary Design Optimization

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Response surface methods have been used for a variety of applications in aerospace engineering, particularly in multidisciplinary design optimization. We investigate the use of kriging models as alternatives to traditional second-order polynomial response surfaces for constructing global approximations for use in a real aerospace engineering application, namely, the design of an aerospike nozzle. Our objective is to examine the difficulties in building and using kriging models to create accurate global approximations to facilitate multidisciplinary design optimization. Error analysis of the response surface and kriging models is performed, along with a graphical comparison of the approximations. Four optimization problems are also formulated and solved using both sets of approximation models to gain insight into their use for multidisciplinary design optimization. We find that the kriging models, which use only a constant “global” model and a Gaussian correlation function, yield global approximations that are slightly more accurate than the response surface models.

Nomenclature

n_s	=	number of sample points
R	=	correlation matrix in kriging model
$R(x^i, x^j)$	=	correlation function between points x^i and x^j
\hat{y}	=	predicted response value at untried x
β	=	constant underlying global portion of kriging model
$\beta_i, \beta_{ij}, \beta_{ii}$	=	linear, interaction, and quadratic coefficients in polynomial response surface
θ_k	=	correlation parameters in kriging model
$\hat{\sigma}^2$	=	variance estimate

I. Introduction: Frame of Reference

MANY engineering analyses rely heavily on running complex computer analysis and simulation codes such as finite element and computational fluid dynamic analyses to simulate the performance of the system under consideration. Depending on the fidelity of these analyses, they can become computationally expensive, limiting optimization and design space exploration. Consequently, statistical approximations are becoming widely used in aerospace engineering to construct simplified approximations, or metamodels, of these analysis codes that are then used in lieu of the actual analysis codes, providing a surrogate model of the original code. By far the most popular technique for building metamodels in aerospace engineering is the traditional response surface method,¹

which typically employs second-order polynomial models fit using least-squares regression techniques. Recent reviews of response surface modeling approaches in aerospace engineering,² structural design,³ and mechanical engineering⁴ are available in the literature and are therefore not repeated here.

Because response surfaces are typically second-order polynomial models, they have limited capability to model nonlinear functions of arbitrary shape accurately. Higher-order response surface models can be used to approximate a nonlinear design space; however, instabilities may arise,⁵ or it is often too difficult to take enough sample points to estimate all of the coefficients in the polynomial equation, particularly in high dimensions. Consequently, many researchers advocate the use of a sequential response surface modeling approach using move limits⁶ or a trust region approach.⁷ For instance, the Concurrent Subspace Optimization procedure uses data generated during concurrent subspace optimization to develop response surface approximations of the design space that form the basis of the subspace coordination procedure.^{8–10} The Hierarchical and Interactive Decision Refinement methodology uses statistical regression and other metamodeling techniques to recursively decompose the design space into subregions and fit each region with a separate model during design space refinement.¹¹ Finally, the model management framework is being developed collaboratively by researchers at The Boeing Company, IBM Corporation, and Rice University to implement mathematically rigorous techniques to manage the use of approximation models in optimization.¹²

Many of these sequential approaches are being developed for single-objective optimization applications; however, much of engineering design is multi-objective, and it is often difficult to isolate a small region of good design that can be accurately represented by a low-order polynomial response surface model. Barton⁵ goes so far as to state that the response region of interest will never be reduced to a “small neighborhood” that is good for all objectives during multi-objective optimization. Koch et al.¹³ discuss the difficulties encountered when screening large-variable problems with multiple objectives as part of the response surface approach. Consequently, there is a need to investigate metamodeling techniques that are capable of generating accurate global approximations of the design space over potentially large regions of interest.

Kriging models show great promise for building accurate global approximations of a design space.¹⁴ These metamodels are extremely flexible because of the wide range of spatial correlation

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functions that can be chosen for building the approximation, provided sufficient sample data are available to capture the trends in the system responses. As a result, kriging models can approximate linear and nonlinear functions equally well. Furthermore, kriging models can either “honor the data,” by providing an exact interpolation of the data, or “smooth the data,” by providing an inexact interpolation.^{15,16} Smoothing numerical noise in a simulation code is one of the many nice features that noninterpolating approximations such as response surface models offer.¹⁷

Unlike response surfaces, however, kriging has found extremely limited use in aerospace engineering since its introduction into the literature by Sacks et al.¹⁴ Many researchers have employed kriging modeling strategies specifically for numerical optimization.^{18–20} Giunta and Waston²¹ perform a cursory investigation into the use of kriging for 1-, 5-, and 10-variable sinusoidal test problems; they observe that the quadratic polynomial models were more accurate than the interpolative kriging models based on several error metrics. Iterative strategies using kriging have also been developed. Booker²² discusses a 31-variable and a 56-variable helicopter-rotor structural design problem, stating that the flexibility of the kriging models allows them to be improved iteratively in regions of interest through intelligent “intervention” of a design expert. Finally, Osio and Amon²³ present a multistage kriging strategy to design an embedded electronic package with five design variables.

The limited use of kriging models in engineering applications may be due to 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 compared with a simple response surface model. Consequently, the objective in this paper is to examine the difficulties in building and using kriging models to create accurate global approximations to facilitate multidisciplinary design optimization. Toward this end, kriging models and response surface models are constructed for an aerospike nozzle design problem to compare their capability in producing accurate global approximations. Their accuracy is compared through numerical error analysis and graphical analysis and their capability to generate accurate solutions for four different optimization problems. The rates with which these solutions are obtained also gives insight into the capability of each type of approximation to facilitate multidisciplinary design optimization. The mathematics for constructing response surface and kriging models are described next.

II. Descriptions of Response Surface Models and Kriging Models

Building approximations of computer analyses involves 1) choosing an experimental design to sample the computer analysis code, 2) selecting an approximation model to represent the data, and 3) fitting the model to the sample data. A variety of options exists for each.⁴ Although choosing an experimental design is an important issue in building approximations, our focus in this paper is on constructing accurate approximations from a given set of sample data; comparisons of experimental design strategies are available elsewhere in the literature.^{24–28} An overview of response surface models is given next, followed by a description of kriging models.

A. Response Surface Models

Response surface modeling techniques were originally developed to analyze the results of physical experiments to create empirically based models of the observed response values.²⁹ Response surface modeling postulates a model of the form

$$y(x) = f(x) + \varepsilon \quad (1)$$

where $y(x)$ is the unknown function of interest, $f(x)$ is the polynomial approximation of x , and ε is random error that is assumed to be normally distributed with mean zero and variance σ^2 . The error, ε_i , at each observation is assumed to be independent and identically distributed. The polynomial function, $f(x)$, used to approximate $y(x)$ is typically a low order polynomial, which is assumed to be either linear, Eq. (2), or quadratic, Eq. (3):

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

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

The parameters, β_0 , β_i , β_{ii} , and β_{ij} , of the polynomials in Eqs. (2) and (3) are determined through least-squares regression, which minimizes the sum of the squares of the deviations of predicted values, $\hat{y}(x)$, from the actual values, $y(x)$. The coefficients of Eqs. (2) and (3) can be found using Eq. (4):

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

where X is the design matrix of sample data points, X' is its transpose, and y is a column vector that contains the values of the response at each sample point. Additional details on least-squares regression response surface modeling can be found in many books.^{1,29,30}

B. Kriging Models

Unlike response surfaces, kriging models have their origins in mining and geostatistical applications involving spatially and temporally correlated data.^{15,31} Kriging models combine a global model plus localized departures:

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

where $y(x)$ is the unknown function of interest, $f(x)$ is the known approximation (usually polynomial) function, and $Z(x)$ is the realization of a stochastic process with mean zero, variance σ^2 , and nonzero covariance. The $f(x)$ term in Eq. (5) is similar to a polynomial response surface, providing a “global” model of the design space. In many cases $f(x)$ is taken as a constant, β ,^{14,28,32,33} and we employ only a constant term for $f(x)$ in the aerospike nozzle design example in Sec. III.

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; however, noninterpolative kriging models can also be created to smooth noisy data.^{15,16} The covariance matrix of $Z(x)$ is given by Eq. (6):

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

In Eq. (6), R is the correlation matrix, and $R(x^i, x^j)$ is the correlation function between any two of the n_s sampled data points x^i and x^j . R is an $(n_s \times n_s)$ symmetric matrix with ones along the diagonal. The correlation function $R(x^i, x^j)$ is specified by the user, and a variety of correlation functions exist.^{33–35} In this paper, we utilize the Gaussian correlation function of the form

$$R(x^i, x^j) = \exp \left[- \sum_{k=1}^n \theta_k |x_k^i - x_k^j|^2 \right] \quad (7)$$

where n_{dv} is the number of design variables, θ_k are the unknown correlation parameters used to fit the model, and x_k^i and x_k^j are the k th components of sample points x^i and x^j . In some cases, using a single correlation parameter gives sufficiently good results^{14,23,36}; however, we use a different θ for each design variable.

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

$$\hat{y} = \hat{\beta} + r^T(x)R^{-1}(y - f\hat{\beta}) \quad (8)$$

where y is the column vector of length n_s that contains the sample values of the response, and f is a column vector of length n_s that is filled with ones when $f(x)$ is taken as a constant. In Eq. (8), $r^T(x)$ is the correlation vector of length n_s between an untried x and the sampled data points $\{x^1, \dots, x^{n_s}\}$

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

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

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

The estimate of the variance, $\hat{\sigma}^2$, between the underlying global model $\hat{\beta}$ and y is estimated using Eq. (11):

$$\hat{\sigma}^2 = [(y - f\hat{\beta})^T R^{-1} (y - f\hat{\beta})] / n_s \quad (11)$$

where $f(x)$ is assumed to be the constant $\hat{\beta}$. The maximum likelihood estimates (i.e., “best guesses”) for the θ_k in Eq. (7) used to fit a kriging model are obtained by solving Eq. (12):

$$\max_{\theta_k > 0} \Phi(\theta_k) = -[n_s \ell_n(\hat{\sigma}^2) + \ell_n |\mathbf{R}|] / 2 \quad (12)$$

where both $\hat{\sigma}^2$ and $|\mathbf{R}|$ are functions of θ_k . While any value for the θ_k creates an interpolative kriging model, the “best” kriging model is found by solving the k -dimensional unconstrained nonlinear optimization problem given by Eq. (12). We employ a simulated annealing algorithm³⁷ to find the maximum likelihood estimates for the θ_k parameters, and the associated computational expense is found to be minimal in the aerospike nozzle design example, described next.

III. Aerospike Nozzle Design Example

The linear aerospike rocket engine is the propulsion system proposed for the VentureStar³⁸ reusable launch vehicle. The aerospike rocket engine consists of a rocket thruster, cowl, aerospike nozzle, and plug base regions as shown in Fig. 1. The aerospike nozzle is a truncated spike or plug nozzle that adjusts to the ambient pressure and integrates well with launch vehicles. The flowfield structure changes dramatically from low altitude to high altitude on the spike surface and in the base flow region. Additional flow is injected in the base region to create an aerodynamic spike, which gives the aerospike nozzle its name, increasing the base pressure and contribution of the base region to the thrust. The aerodynamic and structural analysis for the aerospike nozzle were originally developed by Korte et al.³⁹ and are employed in this paper to compare the accuracy of global approximations based on response surface and kriging models.

The multidisciplinary analysis of the aerospike nozzle involves two disciplines, aerodynamics and structures, and there is an in-

teraction 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 analysis and are linked to a structural finite element analysis model in NASTRAN 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 liftoff weight (GLOW). The corresponding multidisciplinary domain decomposition is illustrated in Fig. 2.

For this study, we consider three design variables for the multidisciplinary design of the aerospike nozzle: starting (thruster) angle, exit height, and length, as shown in Fig. 3. The thruster angle α is the entrance angle of the gas from the combustion chamber onto the nozzle surface; the height h and length l refer to the solid portion of the nozzle itself. A quadratic curve defines the aerospike nozzle surface profile based on the values of thruster angle, height, and length.

Bounds for the design variables are set to produce viable nozzle profiles from the quadratic model based on all combinations of thruster angle, height, and length. Second-order response surface models and kriging models are developed for each of the three system responses (thrust, weight, and GLOW) as described next.

A. Approximations for the Aerospike Nozzle Problem

Sample data for fitting the response surface and kriging models for the aerospike nozzle example is obtained from a 25-point (strength 2) orthogonal array.⁴⁰ The sample data and corresponding response values are summarized in Table 1. The data have been scaled against the baseline design to protect the proprietary nature of the data.

For three reasons, the 25-point orthogonal array is chosen over the traditional central composite design, which contains only 15 sample points for three design variables. First, since each analysis requires 25 to 30 min of computation time, 25 simulation runs can be conveniently completed overnight when computer resources are not

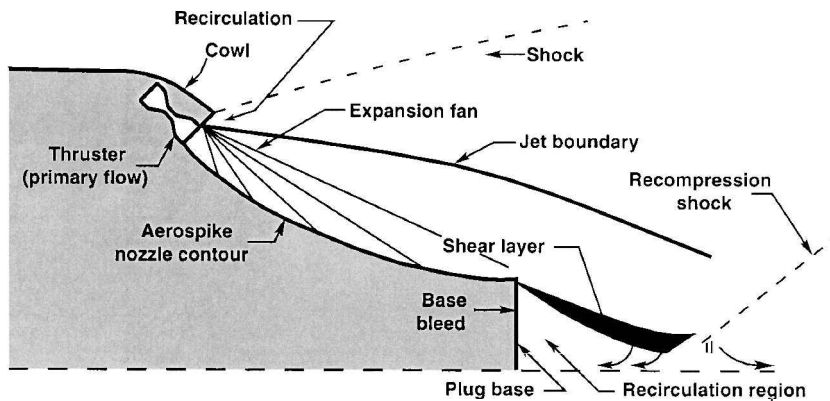


Fig. 1 Aerospike components and flowfield characteristics.³⁹

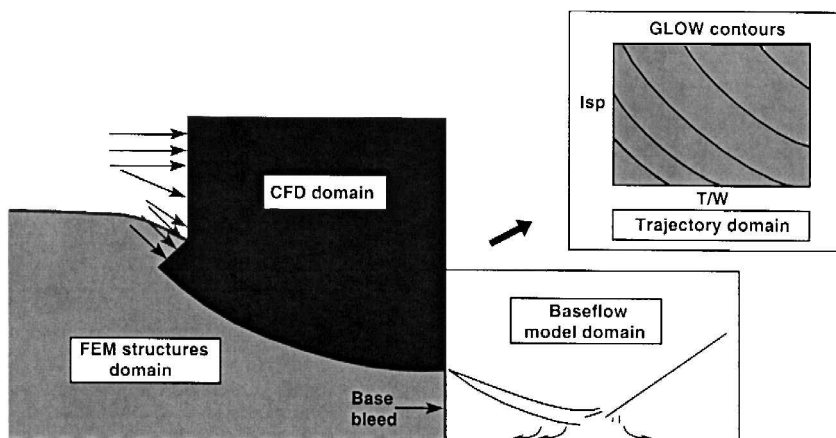


Fig. 2 Multidisciplinary domain decomposition.³⁹

in high demand. Second, Giunta et al.¹⁷ recommend using $1.5n$ to $2.5n$ sample points to produce an accurate response surface model, where n is the number of coefficients that need to be estimated. (For 3 design variables, $n = 10$.) Preliminary approximations based on fewer sample points yielded poor results; therefore, larger sample sizes were allocated because computational resources permitted it. Finally, and most important, we have found that central composite designs frequently lead to singularities in the correlation matrix in Eq. (6) when performing the maximum likelihood estimation as a result of the location and spacing of the sample points in the design space.^{41,42} Therefore, we are investigating space-filling designs such as the strength 2 orthogonal array to provide more accurate surrogate approximations,⁴³ although our objective in this paper is to investigate the use of kriging models to build global approximations based on the given sample data. Toward this end, response surface models for each of the system responses are constructed in Sec. III.B to

provide a basis for comparison against the kriging models that are developed from the same set of sample data in Sec. III.C.

B. Response Surface Models for the Aerospike Nozzle Example

Second-order response surface models for weight, thrust, and GLOW are fit to the 25 sample points by using ordinary least-squares regression. The corresponding response surface models are given in Eqs. (13–15). The resulting R^2 , R^2_{adjusted} , and RMSE (root mean square error⁴⁴) values for each response surface model are listed in Table 2.

Weight = $0.810 - 0.116a + 0.121h + 0.152l + 0.065a^2$
 $- 0.025ah + 0.0013h^2 - 0.0539al - 0.0131hl$
 $+ 0.0301l^2$ (13)

Thrust = $0.9968 + 0.00031a + 0.0019h + 0.0060l - 0.00175a^2$
 $+ 0.00125ah - 0.0011h^2 + 0.00125al - 0.00198hl$
 $- 0.00165l^2$ (14)

GLOW = $0.9930 - 0.0270a + 0.0065h - 0.0265l + 0.0307a^2$
 $- 0.0163ah + 0.0100h^2 - 0.0226al + 0.0151hl$
 $+ 0.0195l^2$ (15)

As evidenced by the high R^2 and R^2_{adjusted} values and low RMSE values in Table 2, the response surface models appear to capture a large portion of the observed variance, indicating a good fit. The kriging models are presented next.

C. Kriging Models for the Aerospike Nozzle Example

For the kriging models, a constant term is used for the underlying global portion of the kriging model and a Gaussian correlation

Table 1 Normalized sample data from orthogonal array

Run number	Design variable			Response		
	Angle	Height	Length	Thrust	Weight	GLOW
1	−1	0	0.5	1.0004	0.9815	0.9924
2	−1	1	1	0.9998	1.1191	1.0214
3	−1	−1	0	0.9993	0.8987	0.9864
4	−1	−0.5	−1	0.9972	0.8422	0.9954
5	−1	0.5	−0.5	0.9987	0.9346	0.9996
6	1	0	1	1.0013	0.9242	0.9714
7	1	1	0	0.9997	0.9090	0.9842
8	1	−1	−1	0.9955	0.7550	0.9947
9	1	−0.5	−0.5	0.9975	0.8028	0.9850
10	1	0.5	0.5	1.0005	0.9166	0.9777
11	0.5	0	0	0.9997	0.8896	0.9805
12	0.5	1	−1	0.9978	0.8632	0.9949
13	0.5	−1	−0.5	0.9976	0.7865	0.9804
14	0.5	−0.5	0.5	1.0006	0.8946	0.9716
15	0.5	0.5	1	1.0013	0.9682	0.9802
16	−0.5	−1	0.5	1.0005	0.9094	0.9759
17	−0.5	0	−1	0.9976	0.8437	0.9916
18	−0.5	1	−0.5	0.9988	0.9328	0.9981
19	−0.5	−0.5	1	1.0015	0.9705	0.9782
20	−0.5	0.5	0	0.9998	0.9421	0.9900
21	0	0	−0.5	0.9988	0.8663	0.9847
22	0	1	0.5	1.0007	0.9604	0.9846
23	0	−1	1	1.0015	0.9266	0.9691
24	0	−0.5	0	0.9997	0.8536	0.9731
25	0	0.5	−1	0.9978	0.8508	0.9915

Table 2 Error diagnostics of response surface models

Measure	Response		
	Weight	Thrust	GLOW
R^2	0.986	0.998	0.971
R^2_{adjusted}	0.977	0.996	0.953
RMSE	1.12%	0.01%	0.25%

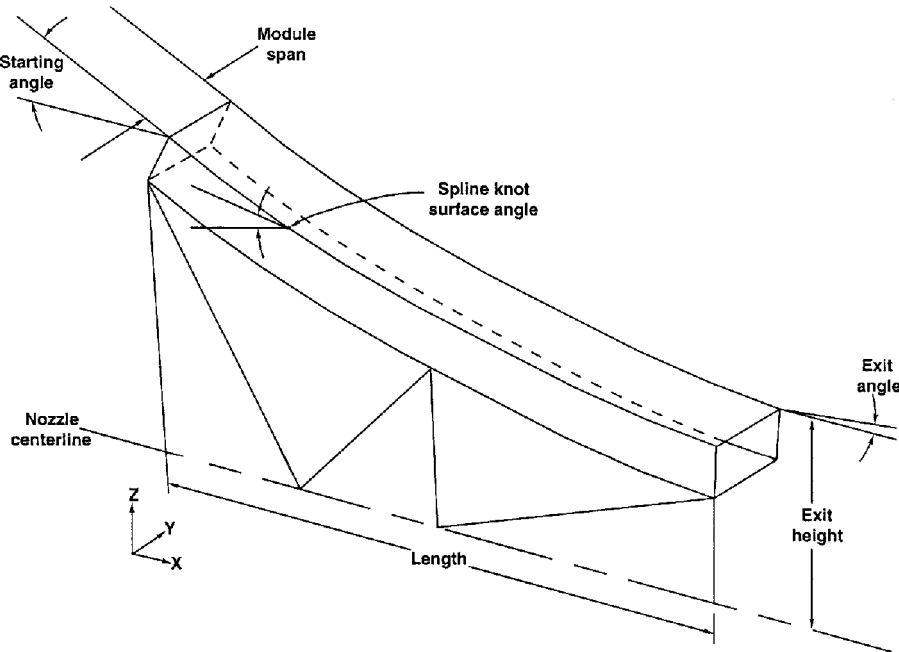


Fig. 3 Nozzle geometry.³⁹

function, Eq. (7), is used for the local deviations. Initial investigations revealed that a single θ parameter was insufficient to model the data accurately when scaling the design variables to $[0, 1]^3$. Therefore, a simulated annealing algorithm³⁷ is used to determine the maximum likelihood estimates (MLEs) for the three θ parameters needed to find the “best” kriging model. The resulting MLEs for the three θ parameters for each kriging model for weight, thrust, and GLOW are summarized in Table 3. Determination of the MLEs for the three θ parameters using the simulated annealing algorithm required approximately 1 min of computation time on a 300-MHz Sun Ultra Sparc60.

With these parameters for the Gaussian correlation function and the 25 sample data points, the kriging models are fully specified. A new point is predicted using these values in combination with Eqs. (8–10), and a comparison of the accuracy of these kriging models and the response surface models is discussed next.

D. Error Analysis of Response Surface Models and Kriging Models

Because the kriging models interpolate the sample data, 25 additional, randomly selected validation points are used to verify the accuracy of the kriging models; the accuracy of the response surface models is also examined using these 25 points. Error is defined as the difference between the actual response from the computer analysis, y , and the predicted value, \hat{y} , from either the response surface model or the kriging model. The maximum absolute percent error, the average absolute percent error, and the RMSE for the 25 validation points are summarized in Table 4.

As seen in Table 4, the kriging models have lower maximum absolute error and lower RMSE values for weight and GLOW than the response surface models. Meanwhile, the response surface model for thrust is slightly better than the kriging models; the maximum error and RMSE are slightly less, and the average errors are essentially the same. It is not surprising that the response surface model predicts thrust better: it has a very high R^2 value (0.998) and low

RMSE (0.01%), as noted previously in Table 2. It is reassuring to note, however, that the kriging model, despite using a constant term and a Gaussian correlation function, is only slightly less accurate than the corresponding second-order response surface model for thrust. In summary, it appears that both models predict well, with the kriging models having a slight advantage in accuracy because of the lower RMSE values. A graphical comparison of the two sets of approximations is offered next.

E. Graphical Comparison of Response Surface Models and Kriging Models

In Figs. 4–7, three-dimensional contour plots of thrust, weight, and GLOW are given. In each figure, the same contour levels are used for the response surface and kriging models so that the shapes of the contours can be directly compared.

In Fig. 4, the contours of the response surface model and the kriging model for thrust are very similar. As evidenced by the high R^2 and low RMSE values, we expect the response surface model to approximate thrust quite well, and it is reassuring to note that the kriging models closely resemble the response surface models even through the underlying global model for the kriging models is only a constant.

The contours of the response surface and kriging models in Fig. 5 are also very similar, but we begin to see localized perturbations due to the fact that the kriging model interpolates the data. The error analysis from the preceding section indicated that the kriging model for weight is slightly more accurate than the response surface model, which might be attributed to these small nonlinear localized variations.

The general shape of the GLOW contours is the same in Fig. 6; however, the size and shape of the different contours, particularly along the length axis, are quite different. The end view of the GLOW

Table 3 Theta parameters for kriging models for scaled data

Parameter	Response		
	Weight	Thrust	GLOW
θ_{angle}	0.549	0.299	3.357
θ_{height}	1.324	0.384	2.518
θ_{length}	2.720	1.866	0.524

Table 4 Error analysis of response surface and kriging models

Model	Weight	Thrust	GLOW
Second order response surface			
Max % error	19.57	0.032	3.68
Avg % error	2.44	0.012	0.53
RMSE, %	4.54	0.015	0.90
Kriging (with constant term)			
Max % error	17.23	0.048	3.43
Avg % error	2.51	0.012	0.59
RMSE, %	4.37	0.018	0.89

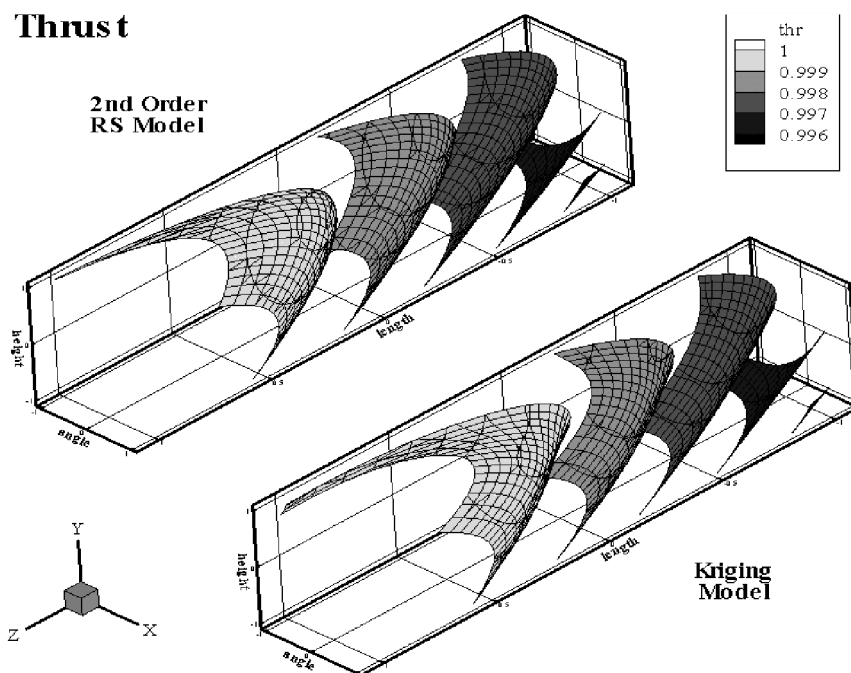


Fig. 4 Thrust contours.

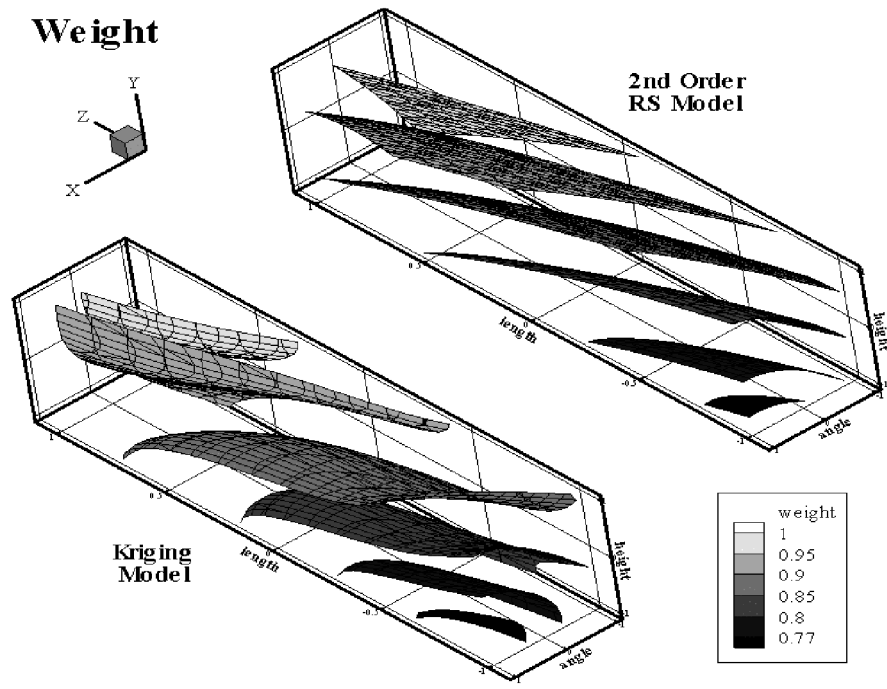


Fig. 5 Weight contours.

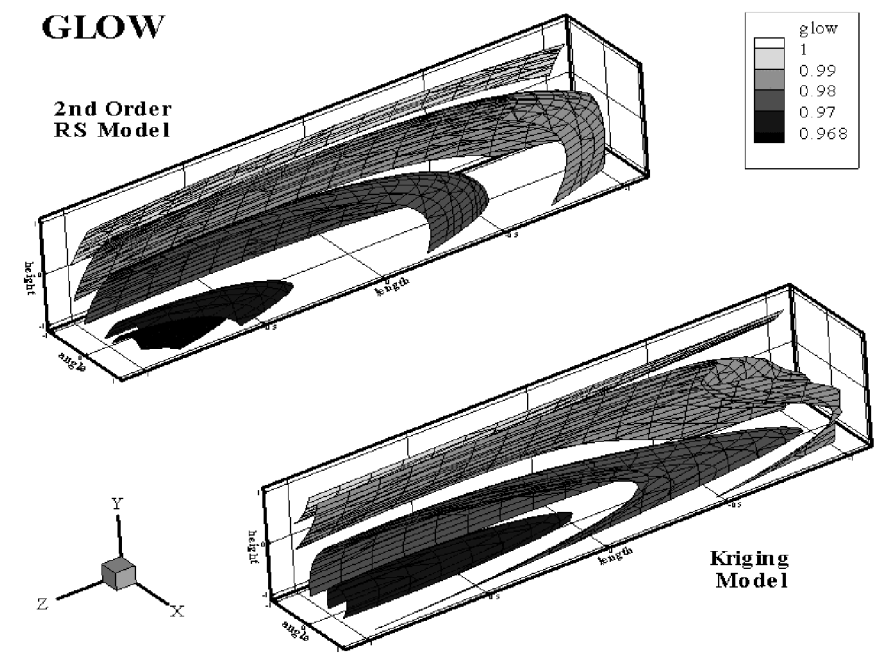


Fig. 6 GLOW contours.

contours along the length axis shown in Fig. 7 further highlights the differences between the two models.

Notice in Fig. 7 that the kriging model predicts a minimum GLOW located within the design space centered around height = -0.8, angle = 0, along the axis defined by $0.2 \leq \text{length} \leq 0.8$. This minimum was verified through additional experiments and found during optimization, as discussed next.

F. Optimization Results Using Response Surface Models and Kriging Models

As a final comparison of the accuracy of the response and kriging models, we formulate and solve four different optimization problems: 1) maximize thrust, 2) minimize weight, 3) minimize GLOW, and 4) maximize thrust/weight ratio, as summarized in Fig. 8. The first two objective functions represent traditional, single-objective, single-discipline optimization problems. The second, two-objective

functions are characteristic of multidisciplinary optimization; minimizing GLOW or maximizing the thrust/weight ratio requires trade-offs between the aerodynamics and structures disciplines. For each optimization, constraints are placed on the maximum and minimum allowable values of responses that are not part of the objective function. For instance, in the first problem, the objective is to maximize thrust subject to constraints on maximum weight, weight_{\max} , and GLOW, GLOW_{\max} , and the minimum thrust/weight ratio, $(\text{Thr}/\text{Wt})_{\min}$, the values of which are hidden to protect the data's proprietary nature.

Each optimization is formulated and solved using the generalized reduced gradient (GRG) algorithm.⁴⁵ Each optimization is solved twice, first using the response surface models and then using the kriging models. Three different starting points (the lower, middle, and upper bounds) are used for each objective function to assess the average number of analysis and gradient calls that is necessary to

obtain the optimum design. The same parameters (e.g., step size, allowable constraint violation) are used within the GRG algorithm for each optimization problem. The results of all four optimizations using both sets of response surface and kriging models are summarized in Table 5, and the following observations are made based on the data in Table 5:

1) Average number of analysis and gradient calls: In general, the optimization requires fewer analysis and gradient calls to the response surface models than the kriging models. This is attributed to the fact that the response surface models are simple second-order polynomials, whereas the kriging models are more complex, nonlin-

ear approximations [see Eqs. (7–10)]. However, the computational expense for both sets of approximations is on the order of milliseconds per evaluation.

2) Convergence rates: Optimization using the response surface models tends to converge more quickly than when using kriging models. This can be inferred from the number of gradient calls, which are one to three calls fewer for the response surfaces than the kriging models.

3) Optimum designs: The optimum designs obtained from the response surface and kriging models are essentially the same for each objective function. The largest discrepancy is the length when

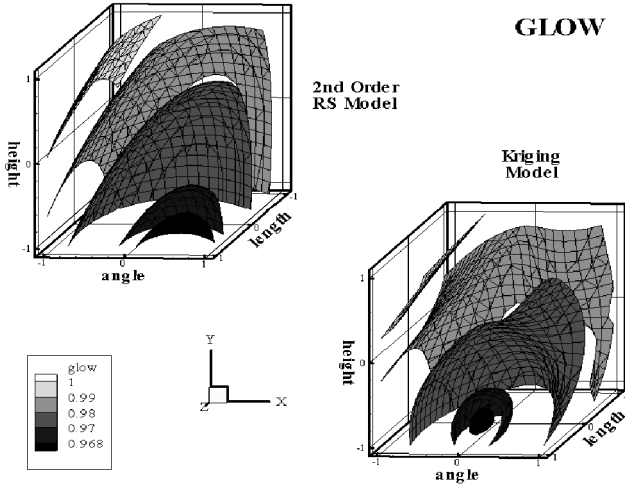


Fig. 7 GLOW contours: end view.

Problem #1: Maximize Thrust	Problem #2: Minimize Weight
Find: $-1 \leq \text{angle} \leq 1$ $-1 \leq \text{height} \leq 1$ $-1 \leq \text{length} \leq 1$	Find: $-1 \leq \text{angle} \leq 1$ $-1 \leq \text{height} \leq 1$ $-1 \leq \text{length} \leq 1$
Satisfy: $\text{Weight} \leq \text{Weight}_{\max}$ $\text{GLOW} \leq \text{GLOW}_{\max}$ $\text{Thr}/\text{Wt} \geq (\text{Thr}/\text{Wt})_{\min}$	Satisfy: $\text{Thrust} \geq \text{Thrust}_{\min}$ $\text{GLOW} \leq \text{GLOW}_{\max}$ $\text{Thr}/\text{Wt} \geq (\text{Thr}/\text{Wt})_{\min}$
Maximize: $\text{Thrust} = f(\text{angle}, \text{height}, \text{length})$	Minimize: $\text{Weight} = f(\text{angle}, \text{height}, \text{length})$
Problem #3: Minimize GLOW	Problem #4: Maximize Thr/Wt Ratio
Find: $-1 \leq \text{angle} \leq 1$ $-1 \leq \text{height} \leq 1$ $-1 \leq \text{length} \leq 1$	Find: $-1 \leq \text{angle} \leq 1$ $-1 \leq \text{height} \leq 1$ $-1 \leq \text{length} \leq 1$
Satisfy: $\text{Thrust} \geq \text{Thrust}_{\min}$ $\text{Weight} \leq \text{Weight}_{\max}$ $\text{Thr}/\text{Wt} \geq (\text{Thr}/\text{Wt})_{\min}$	Satisfy: $\text{Thrust} \geq \text{Thrust}_{\min}$ $\text{Weight} \leq \text{Weight}_{\max}$ $\text{GLOW} \leq \text{GLOW}_{\max}$
Minimize: $\text{GLOW} = f(\text{angle}, \text{height}, \text{length})$	Maximize: $\text{Thr}/\text{Wt} = f(\text{angle}, \text{height}, \text{length})$

Fig. 8 Optimization problem formulation for aerospike nozzle design.

Table 5 Optimization results using response surface and kriging models

Models	Avg. number of analysis calls	Avg. number of gradient calls	Optimum design		Response	Predicted optimum	Verified optimum	% error
Problem 1: Maximize thrust								
RS	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	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	
Problem 2: Minimize weight								
RS	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	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	
Problem 3: Minimize GLOW								
RS	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	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	
Problem 4: 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
			Length	1.000	Thr/Wt	1.0141	1.0173	−0.31
				GLOW	0.9724	1.0228	−4.93	
Kriging	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	

minimizing GLOW. The response surface models predict that the optimum GLOW occurs at the upper bound on length (+1) and the kriging models yield 0.676. This difference is evident in Figs. 6 and 7.

4) 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 error is less than 5% for all cases and less than 0.5% in three quarters of the results.

In summary, the response surface and kriging models yield comparable results for each optimization problem, indicating that both approximation types are equally well suited for multidisciplinary design optimization. In most cases, the kriging models offer slightly more accurate approximations, as evidenced by smaller prediction errors in the optimum design.

IV. Conclusions

In this paper, we have demonstrated the use of kriging models as alternatives to traditional response surface methods for constructing accurate global approximations to facilitate multidisciplinary design optimization. Although the size of the aerospace nozzle design problem is relatively small, only three variables, it provides a realistic aerospace design application in which to compare and contrast the response surface and kriging models. The accuracy of each set of approximations is compared through numerical error analysis, graphical analysis, and their capability to generate accurate solutions for four different optimization problems. We find that the kriging models, using only a constant term for the global portion of the model in conjunction with a Gaussian correlation function, yield global approximations that are slightly more accurate than the response surface models. Furthermore, the rates with which the optimization solutions are obtained gives insight into the capability of each type of approximation to facilitate multidisciplinary design optimization. We find that building and using the kriging models for optimization incur minimal added computational expense and offer predicted optima that are slightly more accurate. These results are promising, but kriging models must be tested on a variety of applications and with a variety of experimental designs before their use becomes as commonplace as that of response surface models in aerospace engineering.

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