Building Aerodynamic Databases Using Enhanced Kriging Surrogate Models

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Recently, we developed a variable-fidelity hybrid Kriging surrogate model[1] that is enhanced by Multivariate Interpolation and Regression (MIR)[2,3] and adaptive training point selection.[4] We use MIR as a local surrogate model that guides the construction of the global Kriging surrogate. The adaptive training point strategy that we use adds training points at locations where the difference between local (MIR) and global (Kriging) surrogate predictions differ by a given threshold.[4] The model is iteratively updated at these locations of greater uncertainty until convergence or a maximum number of evaluations has been reached. This approach helps us to monitor the progress of the surrogate model construction as well as eliminates unnecessary function evaluations in regions where the surrogate is already doing a good job approximating the exact function. In this paper, we demonstrate the use of our hybrid Kriging model for the construction of a two-dimensional aerodynamic database for a NACA 0012 airfoil in steady and inviscid transonic flow. We study the variations of its lift and drag coefficients for changes in Mach number ($0.5 < M < 1.5$) and angle of attack ($0^\circ < \alpha < 5^\circ$). For the purpose of validation of our hybrid surrogate, an "exact" database is obtained through Euler flow solves on a Cartesian mesh of $51 \times 51 = 2601$ equispaced nodes. The root mean square error ($RMSE$) between the exact and surrogate-approximated coefficient values over the entire domain are calculated and used to compare the performances of ordinary Kriging approaches and our enhanced Kriging approach. We also investigate the use of variable-fidelity training points to build the surrogate even more efficiently.

Nomenclature

f	Objective function
$\tilde{f}$	Approximated function value
∇f	Gradient of objective function
x	Sample point location
M	Dimension of sample space
N	Number of training points
N_l	Number of training points for local model
N_t	Number of nodes in M-dimensional Cartesian mesh
n	Taylor order (order of accuracy)

I. Introduction and Motivation

Numerical simulations are extensively used in engineering research to solve real world problems whose analytic solutions are undetermined and in cases where it is impractical to conduct experiments. For example, we do not know an analytic solution for the general Navier-Stokes equations and we are also usually unable to conduct experiments on vehicles operating in hostile and unpredictable environmental conditions (e.g. reentry vehicles) due to technological and financial shortcomings. In these situations, computational methods turn

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out to be very handy and play a key role for aircraft improvements and reductions in development cost and time. Computer simulations have become a mature field, owing to numerous advancements in computational infrastructure including hardware, software and sophistication of numerical algorithms, which have aided in their increased applicability to real life problems. But high-fidelity computational fluid dynamic (CFD) simulations are very expensive in terms of time and they quickly become intractable for higher-dimensional design problems. This computational burden explains the serious need for an alternative for expensive high-fidelity simulations and people have come up with the idea of surrogate models or response surfaces. A surrogate model is an approximate and inexpensive representation of the exact function which - once built - can be interrogated using far less computational time than an exact function evaluation would take. A lot of today's research is directed on improving the accuracy of existing models as well as developing versatile and robust surrogates[2,3,5,6,7] which have captured our attention as well.

One of the key aspects in the engineering design process is the construction of a model (physical or computational) with specified design parameters, testing its performance, and repeating the process until the desired target is achieved. This optimization procedure requires many design iterations (trials) and can be very expensive, thereby prolonging the time span of the whole design process. For example, a relatively straight-forward airfoil optimization can require hundreds if not thousands of flow solutions to reach the optimal design. Moreover, design of complex systems such as airplanes are highly coupled with several disciplines (e.g. propulsion, aerodynamics, structures, controls, etc.) demanding a lot of such optimization processes. Due to each of these time-intensive operations, developing a successful design and its associated production can take a long development time. In these time-constrained situations, it becomes a highly prohibitive practice to test the prototype to obtain the necessary data for design (e.g repeating tests to get lift coefficients of an airfoil), and also due to the difficulties involved with multiple testing and budget cuts. Hence, design teams and agencies have started to focus on building databases that could aid in the design process. Some examples in the literature are listed below:

- Until recently NASA's *Constellation program* was working on a Heavy Lift Launch Vehicle (HLLV) named Ares V, where a simulation protocol was developed to generate databases of the aerodynamic force and moment coefficients for HLLV ascent.[8]
- The NASA Langley Research Center was involved in the development of preflight aerodynamic database of the X-34 Reusable Launch Vehicle (RLV),[9] covering the range of Mach numbers, angles of attack, side-slip and control surface deflections anticipated in the complete flight envelope.
- The Center for Computer Applications in Aerospace Science and Engineering ($C^2A^2S^2E$, part of DLR) is working towards a "Digital Flight" (full flight simulation), for which they develop databases covering the entire flight envelope for many different aircraft configurations.

The increasing demand for efficient and accurate aero-databases has motivated us to pursue this particular research. A key requirement for using CFD in aero-database generation is to establish best practices for accurate and efficient prediction of the force and moment coefficients of the vehicle. In the context of construction of aero-databases, variable-fidelity surrogate model approaches have shown to be very beneficial.[7,10,11,12] Here, the idea is to combine low-fidelity data (e.g. coarser meshes, less sophisticated models) with high-fidelity data (e.g. finer meshes, better models, experimental data). This approach will help us to reduce the time taken to build the surrogate model as the low-fidelity data can be obtained relatively cheap. Recently, we developed a variable-fidelity Kriging surrogate model[1] that is enhanced by Multivariate Interpolation and Regression (MIR)[2,3] and dynamic training point selection.[4] We use MIR as a local surrogate model that guides the construction of the global Kriging surrogate. Our model is a hybrid combining the capabilities of a polynomial-based (MIR) and stochastic method (Kriging) which is expected to perform better than any of these models by themselves. The adaptive training point strategy that we use adds training points at locations where the difference between local (MIR) and global (Kriging) surrogate predictions differ by a given threshold. At these locations exact function evaluations are called and the model is iteratively updated until convergence or a maximum number of evaluations has been reached. We have successfully demonstrated the performance of our hybrid Kriging model on two-, five- and nine-dimensional analytic test functions.[1] A detailed review of our approach is given in Section II.

In this paper, we demonstrate the use of our new model for the construction of a two-dimensional aerodynamic database for a NACA 0012 airfoil in steady and inviscid transonic flow. We study the variations of its lift and drag coefficients for changes in Mach number ($0.5 < M < 1.5$) and angle of attack ($0^\circ < \alpha < 5^\circ$).

An "exact" database is obtained through Euler simulations on a Cartesian mesh of $51 \times 51 = 2601$ equispaced nodes. The root mean square error ($RMSE$) between the exact and surrogate-approximated coefficient values over the entire domain are calculated and used to compare the performances of ordinary Kriging approaches and our enhanced Kriging approach. We also investigate the usage of variable-fidelity training points to efficiently build the surrogate.

Organization of the paper

The remainder of this paper is organized as follows. In Section II, we describe the construction and rationale behind our enhanced Kriging surrogate model guided by MIR and adaptive training point selection. In Section III, we show two-dimensional lift and drag databases that were developed using our model and compare it with the exact database obtained from Euler evaluations. We demonstrate the quality of our enhanced surrogate for these two CFD functionals (lift and drag) using residual plots and compare with ordinary versions of Kriging. We, then show the merit of variable fidelity training points in the surrogate building process and discuss its effectiveness in reducing the total computational time and improving the accuracy of the surrogate. Section IV concludes this paper.

II. Construction of Surrogate Model

In this section, we give a detailed account on the construction of our surrogate model and how we apply it to construct aerodynamic databases. The performance of any metamodel is directly influenced by the non-linearity of the original function, sampling strategies, and types of metamodels, and hence we shall now discuss these concepts briefly.

II.A. Training point selection

The location and number of training points used to construct the surrogate has a significant effect on the accuracy of the model. Thus, we briefly review the available training point selection strategies and outline the merits and demerits associated with them. Sampling approaches can be broadly classified into domain-based and response-based approaches.[13] In domain-based approaches, training points are chosen based on the information available from the design space (e.g. distance between two sample points), whereas in response-based approach, the sample points are chosen based on the information provided by the surrogate model (e.g. mean squared error approach). The latter was developed to enhance the efficiency of the sampling process by using the information from the existing model. For example, in the response-based approach the user could monitor the progress of the model and choose to stop or extend the sampling process. Domain-based sampling is based on space-filling concepts that try to fill the design space evenly with sample points. It is, in general, not possible for the user to select the number of sample points to ensure a given accuracy apriori, due to the non-linearity of most functions of interest. Thus, domain-based approach can be used as an initial sampling before using a sequential sampling. We now review some important domain- and response-based approaches from the literature.

Domain-based approaches

Delaunay Triangulation: Delaunay triangulation is a geometrical method of sampling, where the design space is divided into hyper-triangles and the samples are chosen at some geometrical significant location such as the centers of the hyper-triangles and midpoints of the edges as shown in Figure 1. A major drawback of the Delaunay triangulation is that it does not scale well to higher dimensions.[4]

Monte Carlo: Monte Carlo (MC) techniques[14] are the simplest of all sampling methods. Here, a random number generator is used to select sample point locations in the design space. A major drawback of MC is the fact that for a small amount of sample points large areas of the design space may be left unexplored while others may be sampled densely.[15,16,17]

Latin Hypercube: Latin hypercube sampling (LHS) was proposed by McKay *et al.*[18] for designing computer experiments as an alternative to MC sampling techniques. The basic idea is to divide the range of each design variable into N bins of equal probability, which yields N^M bins in the design space, where M is the dimension of the problem. Subsequently, N samples are generated for each design variable such that

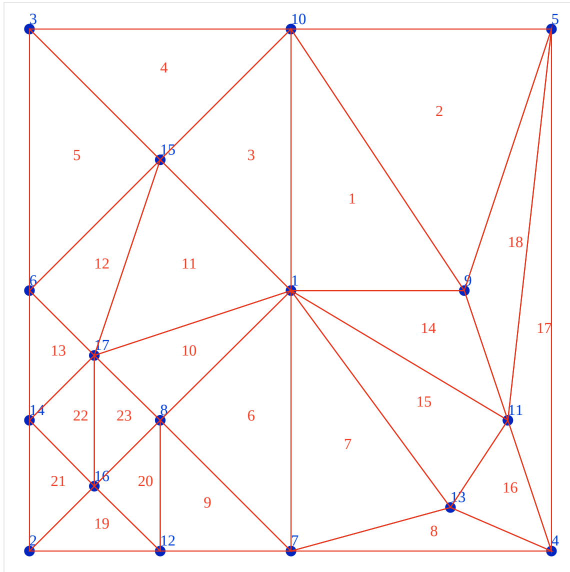

Figure 1. A Delaunay triangulation schematic is shown here. Points numbered 1 to 5 are the initial sample points and 12 points have been added subsequently by splitting the design space into triangles.

no two values lie in the same bin (as shown in Figure 2 (Left)). The LHS algorithm generates samples in a box-shaped domain as follows,[16]

$$x_j^{(i)} = \frac{\pi_j^{(i)} + U_j^{(i)}}{N}, \quad \forall \quad 1 \le j \le M, \quad 1 \le i \le N \tag{1}$$

where $x_j^{(i)}$ is the jth-component of the ith-sample point, $U \in [0, 1]$ is an uniform random number, and π is an independent random permutation of the sequence of integers $0, 1, \ldots, k-1$.

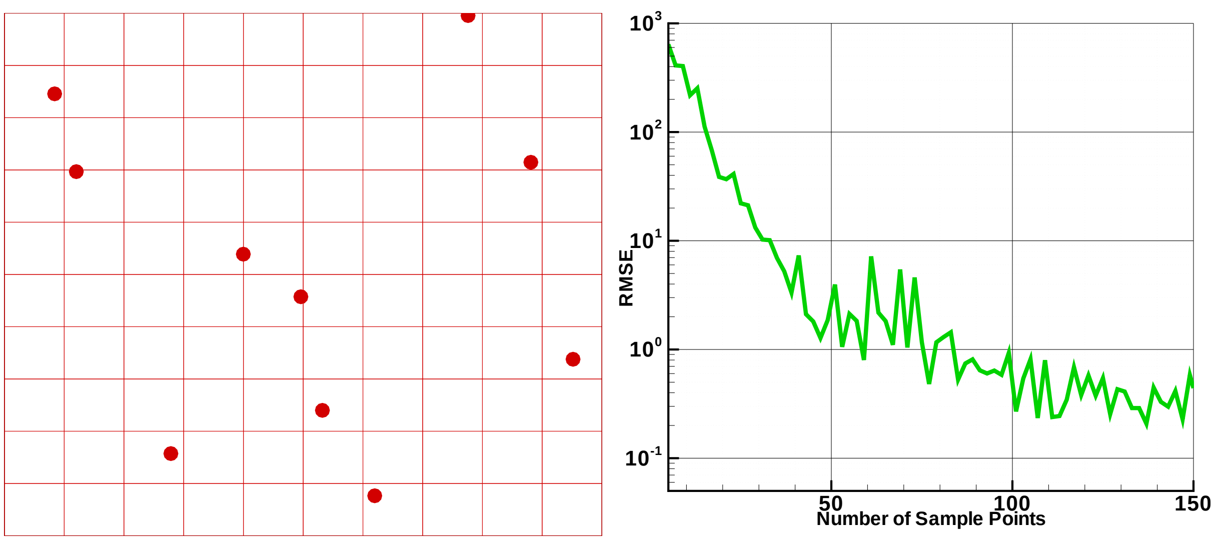

Figure 2. Left: An example of latin hypercube sampling of a two-dimensional design space, where if one-dimensional projections of each design variable are taken, there will be exactly one sample in each bin. Right: A typical convergence history using latin hypercube sampling.

In the right of Figure 2, one can notice the random fluctuations in $RMSE$ of a generic surrogate model based on LHS. At about 50 points, the RMSE is of the order of 10^0 and at about 100 points, the RMSE is still of the order of 10^0. In spite of increasing the number of sample points, the RMSE does not decrease, because all these points are picked at random. If each one of the data-points is from a high fidelity simulation which can take days to run, the situation becomes even worse. This is when one needs a good strategy for training point selection to ensure that the error will reduce when one increases the number of sample points.

Response-based approaches

A brief overview of some important response-based approaches is given in the following paragraphs.

- Jones and Schonlau[19] proposed a sequential response surface methodology which starts with a smaller number of training points and adds additional training points at locations where the standard error is high. During this process, the sample set is updated, the metamodel is reconstructed, and the process of choosing new additional training points continue until the expected improvement from new training points has become sufficiently small.

- Alexandrov[20] proposed a metamodel management framework using a trust-region method for updating metamodels according to the improvement of objective function during an optimization procedure.

- Messac *et al.*[21] developed a new methodology to quantify the surrogate error in different regions of the design space, which is called the Regional Error Estimation of Surrogate (REES) method. The REES method provides a model independent error measure that does not require any additional function evaluations. It works roughly as follows: after segregating the design space into sub-spaces (or regions) variation of the error with sample points (VESP) regression models are constructed to predict the accuracy of the surrogate in each subspace. These regression models are trained by the errors (the mean and the maximum error) evaluated for the intermediate surrogates in an iterative process. At each iteration, the intermediate surrogate is constructed using different subsets of training points and tested over the remaining points. Their results indicate that the REES measure is capable of evaluating the regional performance of a surrogate with reasonable accuracy and that one could use this error estimate to guide the surrogate-building process.

- Rosenbaum *et al.*[22] applied an adaptive sampling strategy where the samples are generated sequentially as well. At every stage of the adaptation process, a surrogate model is generated and assessed in order to find a new training point location at which the objective function is evaluated.

- Recently, a dynamic sampling approach developed by one of the authors[4] has proven to yield better results than other domain-based sampling strategies, where a local surrogate (Dutch Intrapolation) has been employed to guide the training point selection process. First, an initial number of training points are chosen via LHS and more training points are added in locations with the largest discrepancy between the function predictions of the Kriging and the local surrogate model. Thus, instead of just specifying the number of training points in the beginning and picking the points randomly the model is built by adding more training points in promising regions of the design space. This is similar to the concept of expected improvement[19,23] (EI) when optimizing with a Kriging model where a potential for improvement is used, which considers both estimated function values and uncertainties in the surrogate model, thereby keeping the balance between global and local search performance.

- As an extension, the dynamic sampling method has been tested by us with Multivariate Interpolation and Regression[2,3] as local surrogate and has proved to produce even better results.[1] We will use this approach in this paper for the construction of aerodynamic databases.

For a comprehensive review on training point selection strategies the reader is referred to Arora,[13] Keane and Nair,[16] and Forrester *et al.*[17]

II.B. Surrogate model review

In the following paragraphs, short accounts on Kriging and Multivariate Interpolation and Regression are provided, followed by a discussion on the adopted training point selection strategy in this paper.

Kriging

The Kriging model was originally developed in the field of geological statistics by the South-African mining engineer *Danie G. Krige*.[24] Kriging was introduced in engineering design following the work of Sacks *et al*[25] and has been increasingly used in aerospace engineering and design.[26,27,28,29] Kriging predicts the function value by using stochastic processes and has the flexibility to represent multi-modal and non-linear functions.

The basic formulation of Kriging is given as,[13]

$$\tilde{f} = f(x)^T \beta + Z(x) \tag{2}$$

where the first term, $f(x)^T$, models the mean behavior using a regression model and the term, $Z(x)$ models the local variation from the mean behavior using a Gaussian process with zero mean $E[Y(x)] = 0$. For a detailed review on Kriging the reader is referred to Forrester *et al.*[17]

Multivariate Interpolation and Regression

Multivariate Interpolation and Regression (MIR) is a surrogate model where each data point is represented as a Taylor series expansion, and the higher order derivatives in the Taylor series are treated as random variables. The approximation coefficients are then chosen such that they minimize the objective function in each point by solving an equality constrained least squares problem. The approximation is an interpolation when the data points are given as exact, or a non-linear regression function if non-zero measurement errors are associated with the data points. Mathematically, the objective function, f, in an M-dimensional design space is approximated as[2,3]

$$\tilde{f} = \sum_{i=1}^{N_v} a_{vi}(x) f(x_{vi}) + \sum_{i=1}^{N_g} a_{gi}(x) \nabla f(x_{gi}). \tag{3}$$

The tunable parameters in MIR are the Taylor order n, the wave number β, magnitude of the weights γ and polynomial exactness parameter P. We would expect to improve the accuracy of the model by using a higher n, but round-off errors originating in the solution of the least squares problem propagate to the approximate function via Equation (3).

Choice of local and global surrogate

Though, MIR generally produces a more accurate surrogate than Kriging for the same amount of training points, we do not use it as a global surrogate for the following reasons:

1. MIR has severe demerits in terms of computational time that increases rapidly with the number of training points and with the dimensionality of the problem.
2. The existence of tunable parameters, e.g. the choice of an optimum Taylor order n is a tedious task and it varies from function to function and with the dimensionality of the problem as well.
3. Kriging supports the usage of both high- and low-fidelity training points.[10,11,7,12]
4. Kriging has the capability to represent multi-modal functions.[5]

II.C. Construction of our MIR Enhanced Kriging Model

We use a dynamic training point selection strategy by employing MIR as the local surrogate. Figure 3 shows a schematic diagram of our enhanced surrogate construction approach. The steps involved in the process are given below.

- Start by evaluating the function value at the center of the domain.
- Then pick a user specified additional amount of training points via latin hypercube sampling and evaluate their function value.
- Then repeat the following steps until convergence or until a maximum amount of function evaluations has been reached. (We define convergence as having the worst discrepancy below a certain threshold.)
    1. Specify a set of test candidates via latin hypercube sampling.
    2. Construct a local function value for each test candidate using MIR involving an appropriate number of closest neighbors with function information.
    3. Compare the global Kriging surrogate model function value predictions for the test candidates with MIR predictions.

4. Add a user-specified number of test candidates with the worst discrepancy between the two predicted values to the set of training points and evaluate the real function at these discrepant points and rebuild the Kriging surrogate.

- We also augment the selection process by geometric criteria, for example, we make sure that the distance of a test candidate to the nearest existing training point is above the average distance between all test candidates to their respective closest training point. This ensures that the training points are not clustered in one particular region and are sparse in other regions of the design space.

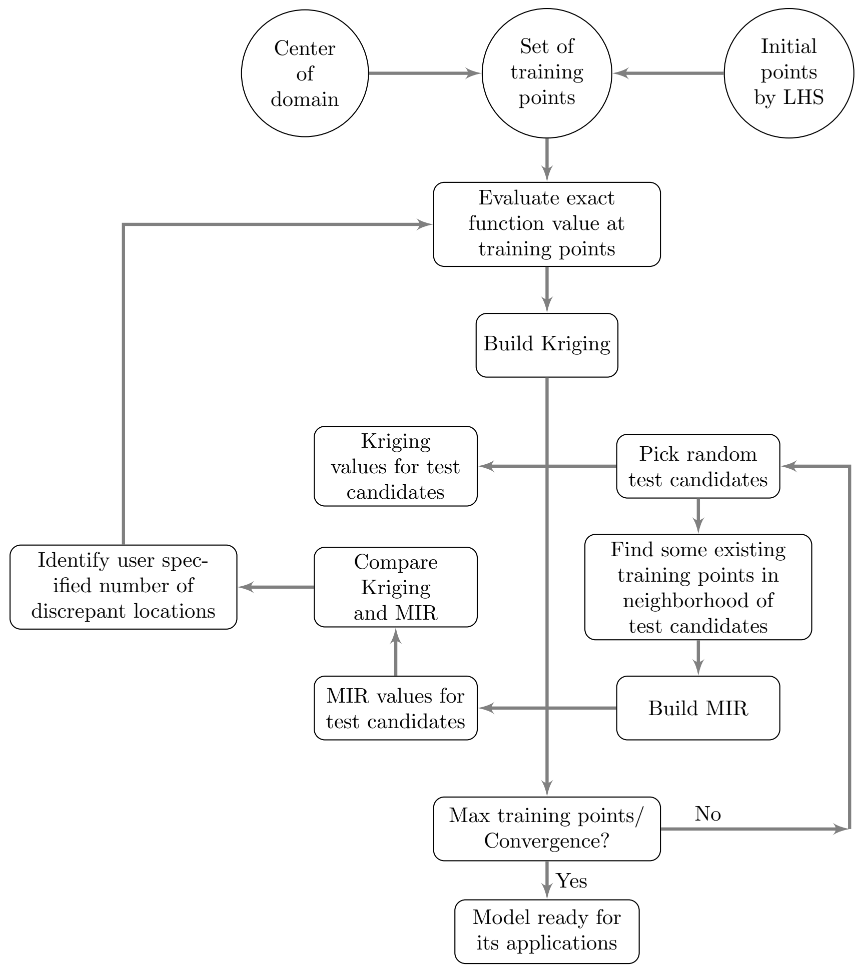

Figure 3. Our enhanced surrogate construction algorithm using MIR as local surrogate

II.D. Validation Methodology

In order to assess the performance of our Kriging surrogate model, we compare it with that of original Kriging and Kriging with Dutch Intrapolation (DI) as a local surrogate.[4] For more background on DI the reader is referred to previously published papers in the literature.[1,4] For each of the three test cases, the root mean square error ($RMSE$) is used as a measure of goodness, and is calculated between the actual, f, and approximated function values, $\tilde{f}$, on an M-dimensional Cartesian mesh with N_t nodes, given as,

$$RMSE = \sqrt{\frac{1}{N_t}\sum_{i=1}^{N_t}(f_i - \tilde{f}_i)^2}, \tag{4}$$

where f_i and $\tilde{f}_i$ are the values in sample point location x_i, $i = 1\ldots, N_t$.

Test Case

The steady inviscid flow around a NACA0012 airfoil is solved by using a cell-centered second-order accurate finite-volume approach.[30,31] The governing inviscid Euler equations are solved on a computational mesh with 19,548 elements shown in Figure 4. We study the variations of the lift and drag coefficients with changes in Mach number ($0.5 < M < 1.5$) and angle of attack ($0° < \alpha < 5°$). The low-fidelity data is calculated on a mesh with only 4,433 elements (not shown), which is roughly four times cheaper to solve than the shown mesh on which the high-fidelity data is calculated. Since, the design space is quite noisy we restrict ourselves from the use of gradients in this paper.

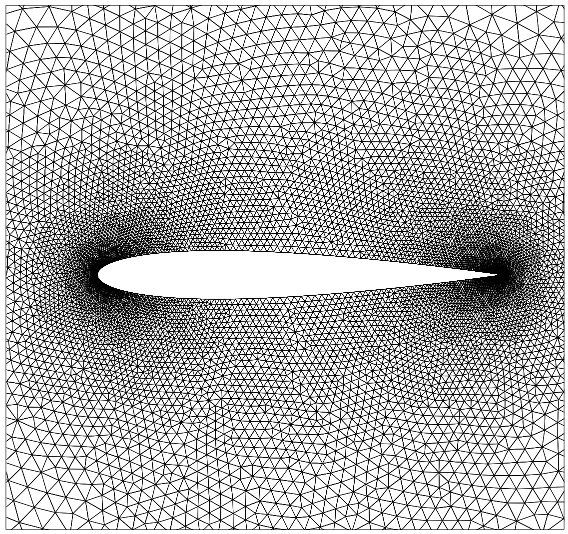

Figure 4. Computational mesh around NACA0012 with about 19,548 elements.

III. Results

In this section, we first compare the convergence behavior of our hybrid Kriging surrogate with other available versions of Kriging. Then we discuss the quality of the aerodynamic database obtained using the surrogate. Finally, we demonstrate the usage of variable fidelity training points in the database building process.

III.A. Convergence Histories

Figure 5 shows the convergence histories of two functionals, namely the drag (left) and lift (right) coefficients. One can see that our enhanced Kriging (shown as blue line) shows better results than other surrogate approaches, namely the original Kriging (shown as green line) and the Kriging enhanced with DI (shown as red line). It can also be inferred that the dynamic training point selection performs better than just selecting all training points through latin hypercube sampling. The dynamic training point selection also helps to reduce the effect due to randomness that more training points do not necessarily lead to a more accurate surrogate model. Another important feature that can be generally observed is that the Kriging with MIR tends to have a better convergence rate than the other two approaches. It can also be seen that dynamic sampling with Dutch Intrapolation performs initially better than our method with MIR. This can be explained as follows. MIR has initially only a few training points around each test candidate and hence is not able to efficiently guide the training point selection process. But as the number of training points increases MIR firmly establishes itself as a better local surrogate than DI, as it now has a sufficient number of data points to build an accurate local approximation.

III.B. Aerodynamic Database of Drag and Lift Coefficients

Figure 6 shows the contour plots of the drag and lift coefficients obtained using Euler flow solves on a Cartesian mesh of $51 \times 51 = 2601$ equispaced nodes and the enhanced Kriging model built using 25 Euler

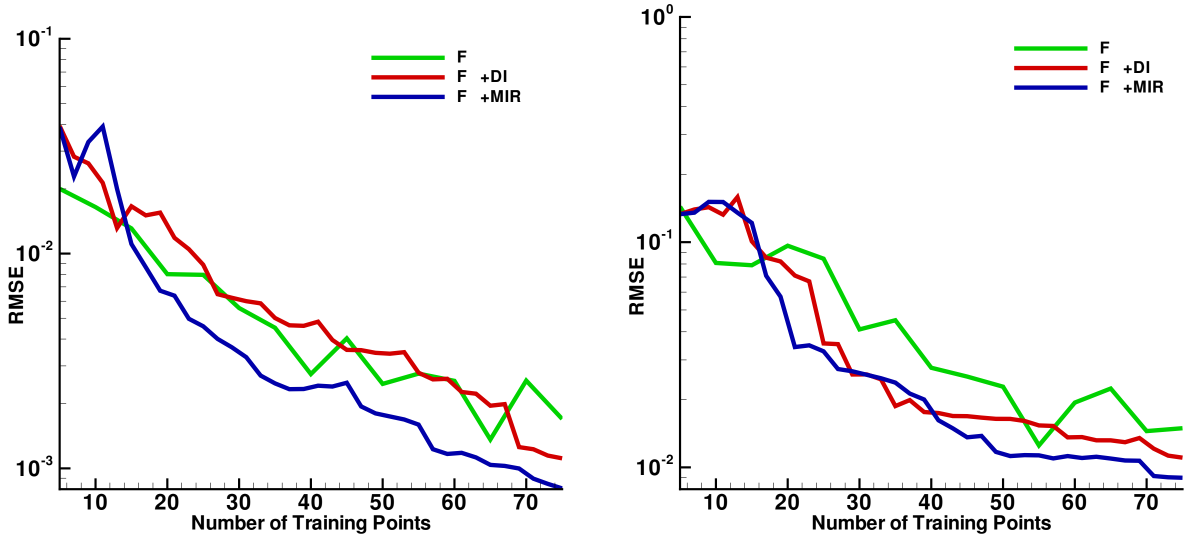

Figure 5. RMSE plotted versus the number of training points for original Kriging (green line), Kriging with Dutch Intrapolation (red line) and our hybrid Kriging with MIR (blue line) for the drag (left) and lift (right) coefficient.

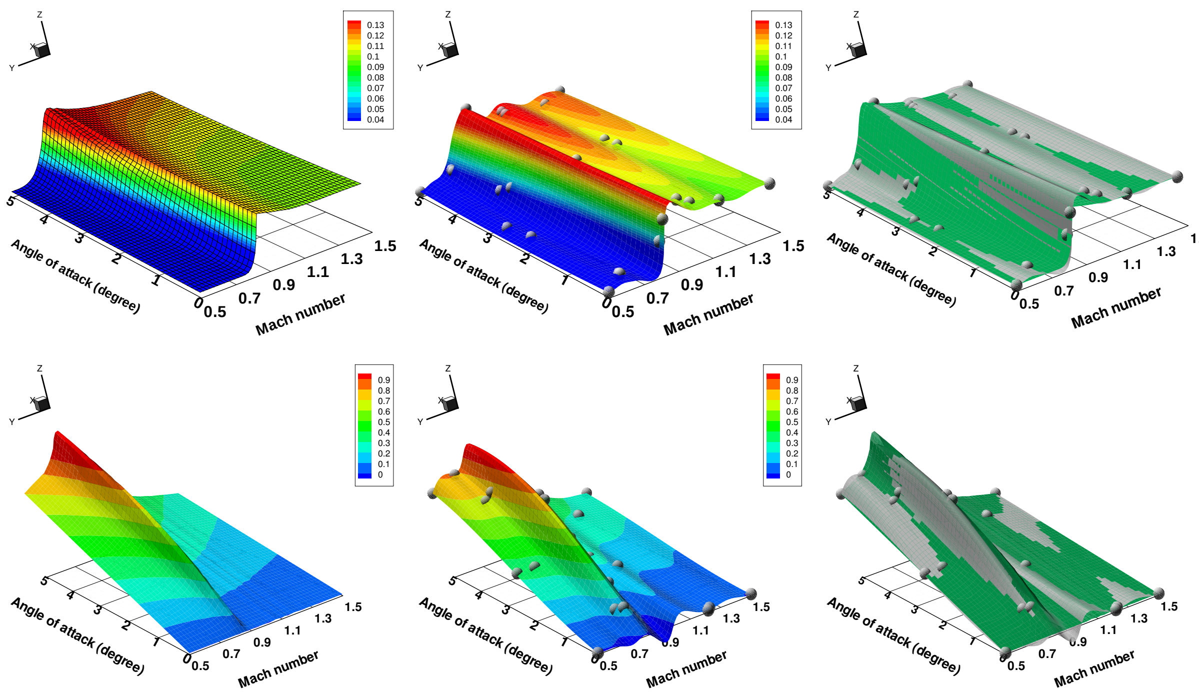

Figure 6. Top: Hyper-surfaces of drag coefficient. Bottom: Hyper-surfaces of lift coefficient. Left: Exact function, Middle: Our Kriging approximation, Right: Both are overlapped, where the green surface is the exact function and the white surface is the Kriging model. The training point locations are shown as gray spheres on the Kriging model's surface.

flow solves. We can see from the depth of the contours that our hybrid Kriging model is in good agreement with the exact model. Our Kriging is able to capture the transonic behavior even though we use way fewer Euler function evaluations, which explains Kriging's popularity in representing highly non-linear functions.

III.C. Variable Fidelity Model

Figure 7 shows the results obtained using variable-fidelity data points. We used 9 high-fidelity and 64 low-fidelity training points for drag, and 15 high-fidelity and 40 low-fidelity training points for lift. We used

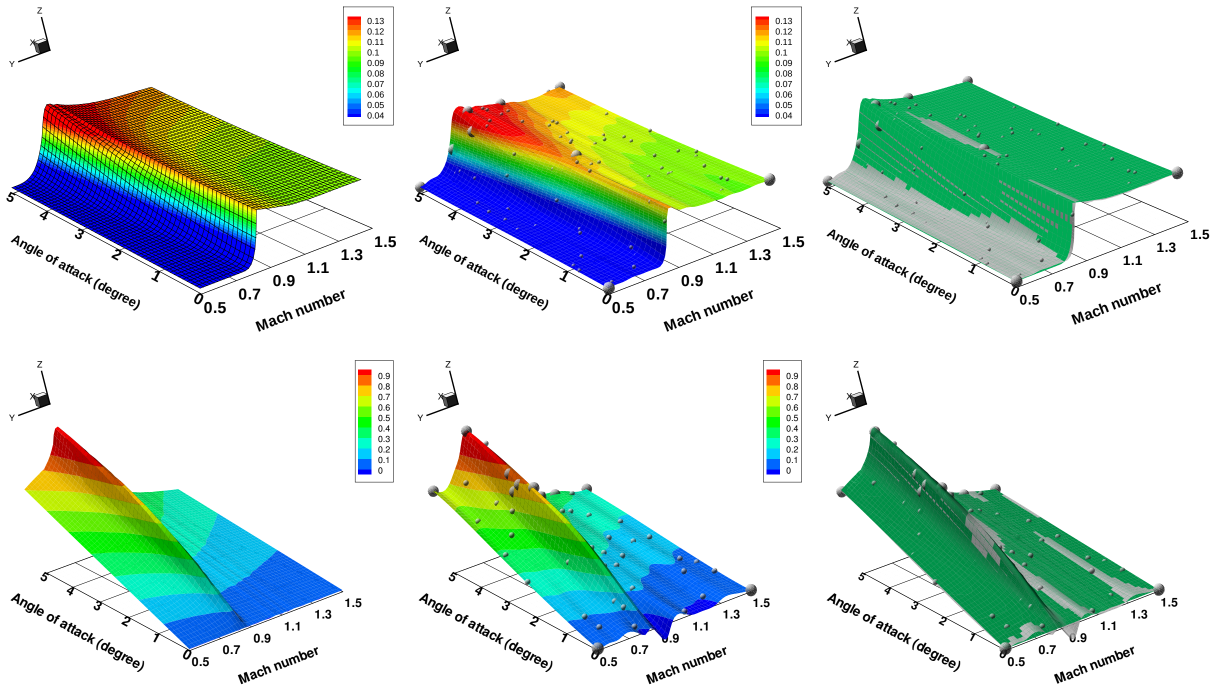

Figure 7. Top: Hyper-surfaces of drag coefficient. Bottom: Hyper-surfaces of lift coefficient. Left: Exact function, Middle: Our Kriging approximation, Right: Both are overlapped, where the green surface is the exact function and the white surface is the Kriging model. The training point locations are shown as gray spheres (the larger ones are the high-fidelity training points and the smaller ones are the low-fidelity training points).

more high-fidelity training points for the lift case, because of the high non-linearity in the transonic flow regime. However, in both the cases, the computational cost is equivalent to that of 25 high-fidelity training points, whose results are shown in Figure 6. One can notice (compare Figures 7 and 6 as well as Table 1) an improvement in the way the variable-fidelity Kriging captures the contour levels for roughly the same computational cost.

Table 1. RMSE comparisons for Kriging models

RMSE	High-fidelity	Variable-fidelity
Drag Coefficient	0.45868×10^{-2}	0.38118×10^{-2}
Lift Coefficient	0.32746×10^{-1}	0.27735×10^{-1}

IV. Conclusions

In this paper, we discussed our hybrid surrogate construction process which uses MIR as local guidance in choosing the training points. Then, we compared the performance of our hybrid Kriging surrogate with other existing Kriging surrogate models and showed that our model performs better for these practical CFD problems, hence it has a great potential for applications in uncertainty quantification and optimization under uncertainty. We compared hyper-surfaces of lift and drag coefficients obtained from Euler solves, with the ones from our enhanced Kriging model and proved its ability to capture highly non-linear behavior making it suitable for CFD applications. Since our model was able to represent the exact behavior with only a very limited number of data points, we are also optimistic that it has great potential to be used for higher-dimensional database constructions and not only the two-dimensional database that we have shown in this paper. Finally, we showed the advantage of using variable fidelity data in the construction of our surrogate, where for roughly the same computational cost a better model is developed.

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