# A Framework for Surrogate-Based Aerodynamic Optimization

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## Abstract

At DLR, an optimization framework combining different CFD solvers, Design of Experiment methods, optimization algorithms, and various surrogate modeling methodologies with sample refinement strategies for efficient surrogate-based global optimization is under development. Several Kriging predictors are used because of their ability to approximate multi-dimensional, highly-nonlinear functions. In order to find global optima accurately, the surrogate model is adaptively refined based on the Kriging error and the Expected Improvement Function. With this hybrid refinement strategy, only a few initial samples need to be evaluated, which improves the performance of the overall optimization process. Additionally, the strategy of running a local optimizer starting from the "optimum" found on the surrogate model is investigated in order to further improve the efficiency and accuracy of the framework. Two test cases indicate that the developed framework combined with hybrid strategy is more efficient.
Keywords: Surrogate-based optimization, Optimization framework, Refinement strategy, Surrogate Model (SGM)

## I. Introduction

At present, aerodynamic optimization plays a quite important role in the research field of aeronautics. On the algorithmic side, traditional optimization methods can be classified into two categories: gradient-based optimization methods and non gradient methods such as genetic algorithm. Gradient-based optimization is a local method, which is faster; at the opposite extreme, genetic algorithms are global optimization methods which require a large number of flow simulations. With the fast development of computer technology, global optimization offers an alternative to designers, simultaneously providing more accurate, rational and intuitional results. Considering time-consuming high-fidelity simulation tools such as Computational Fluid Dynamics (CFD) solvers or Computational Structure Mechanics (CSM) solvers, there still exist serious limitations for applying global aerodynamic optimization. One way of overcoming the defects is to generate a surrogate model by using a few high-fidelity results or high-fidelity results bridged with low-fidelity results, and use it as a predictor instead of the flow solver at an unobserved location in the design space.

At DLR, an optimization framework combining different CFD solvers, Design of Experiment (DoE) methods, optimization algorithms and various surrogate modeling methodologies with sample refinement strategies for efficient surrogate-based global optimization is under development. Figure 1 presents the flowchart of this surrogate-based hybrid optimization strategy. DoE methods are used to generate random samples in the design space, from where the date to be collected contains the information and the attributes of the design space as much as possible. At each sample position, a flow solver is run to obtain the flow solutions, which are used to calculate the objective function at this sample in order to fill a database to construct the surrogate model. Until now in view of the problem to be handled, several Kriging predictors have been integrated because of their ability to approximate multi-dimensional, highly-nonlinear functions [1-3]. Adaptive refinement based on the Kriging Error (KE) and the Expected Improvement (EI) function is used in order to find global optima accurately [4-5]. By using this hybrid refinement strategy, only a few initial samples need to be evaluated, to improve the performance of the overall optimization process. Moreover, the strategy of running a local optimizer starting from the "optimum" found on the surrogate model is investigated in order to further improve the efficiency and accuracy of the framework.

The framework is programmed in Python, correspondingly, the interfaces between different modules and the core executing scripts are also written in Python. Meanwhile, each module in the framework could be used as an independent tool to perform different tasks. Due to the fact that some functions in the module are written in C code, SWIG is used to wrap these C functions with the aim of keeping independency, flexibility and excellent update-performance of each shape.

There are two test cases in this paper. The first one deals with optimization of a NACA 4-digit airfoil with two design variables in transonic flow. An artificial objective function with two optima is constructed by using the lift, drag and moment coefficient. It works as a basic case to test the hybrid chain, efficiency, accuracy and global optimization performance of the framework. The second deals with optimizing the drag of an NLF0416 airfoil with 10 design variables. The transition point is predicted by using the transition module in the DLR TAU code [6-7].

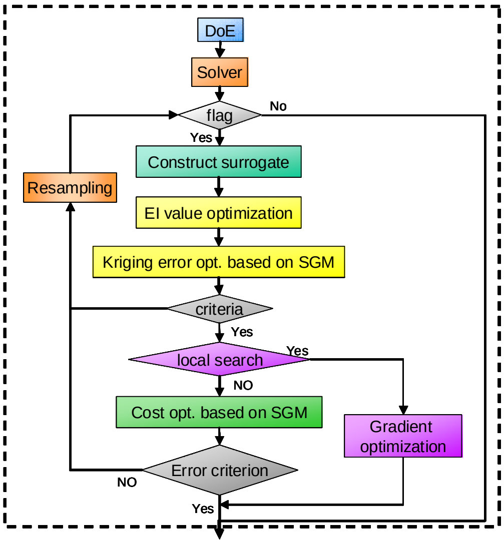



**Figure 1. Flowchart of the surrogate-based hybrid optimization strategy**

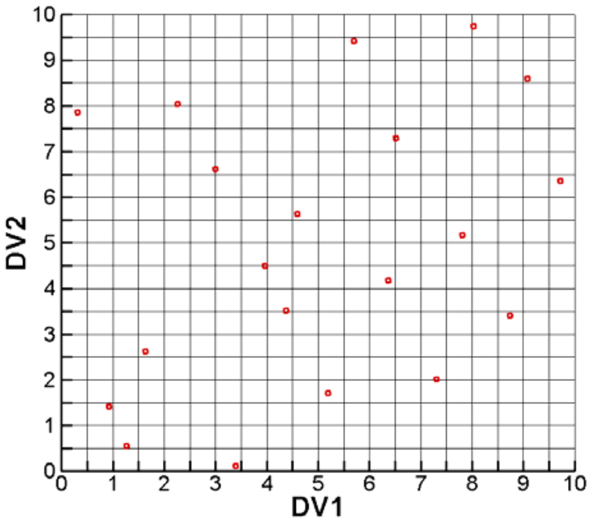



**Figure 2. A DoE plan for 2 dimensional problem with 20 samples**

## II. Design of Experiments (DoE)

Implementing surrogate modeling in optimization depends critically on DoE methods and the chosen surrogate modeling methodologies. DoE is the sampling plan in the design space with the goal of extracting as much information as possible from a limited set of laboratory or computer experiments [3, 8]. The advantages of applying DoE are: require less computer resources, estimate effects of each design variables more precisely, systematically estimate interaction between design variables and acquire global information of the design space [9]. DoE methods are traditionally classified into two categories: classical DoE and modern DoE. Because of dealing with the deterministic computer simulation, modern DoE methods are chosen as the methods in DoE module of the present framework. Up to now, the DoE module consists of Quasi Mont Carlo (QMC) [10], Pseudo Mont Carlo (PMC) [10], Latin Hypercube Sampling (LHS) [11], Optimized Latin Hypercube [12] and Transport Propagation Latin Hypercube (TPLH) [13].

LHS was the first type of DoE method proposed for computer experiments. For the test cases in this paper, LHS is chosen as the DoE method because of its randomness and capacity of the information from the design space. The algorithm is explained in detail in reference [14]. An example of a DoE plan for a two dimension problem with 20 samples by using LHS is shown in

Figure 2.

# III. Shape parameterization and CFD solvers

Different version of the DLR CFD solvers in TAU [15] can be used in the framework to do CFD calculation, such as a low-fidelity Euler solver and a high-fidelity N-S solver. Furthermore, a transition module has been integrated into the framework to predict the transition point [16], and adjoint solver [17] has also been coupled into this tool which could be used to calculate gradients.

If the design variables describe the geometry, a new grid of the geometry needs to be generated in each optimization step. In that case, the TAU deformation tool “deformation” can be used to generate a new grid, provided the old grid and the new geometry are given. If the change of the geometry is not quite large, TAU deformation based on Radial Basis Function (RBF) [18] can be chosen.

At present, there are two parameterization tools inside the framework. The first one is specifically for the NACA 4-digit airfoil based on the analytical functions describing the geometries of the NACA series airfoils [19]. Three values can separately be set as the design variables, the position of the maximal camber, the maximal camber and the thickness of the airfoil. The second one is based on an in-house parameterization tool box called GenGeo. Within the tool box, the bumps of the control points for the geometry can be set as design variables, but the positions of the control points along the x-axis should first be defined and kept unchanged.

# IV. Surrogate modeling and refinement strategies

## A. Surrogate modeling

Kriging is a mathematical method based on statistics, which is used to interpolate the value of a random field at an unobserved location using observation at nearby locations. This idea was originally proposed by Daniel Krige and firstly applied by Sacks et al the deterministic computer simulations in 1989 [20-21]. This technique can be used in practical analyses of the distribution of the value with a known set of values and the correlations between the known values.

Several Kriging such as simple Kriging, ordinary Kriging, universal Kriging, regression Kriging and Gradient Enhanced Kriging (GEK) have been coupled into the framework in view of their ability to approximate multi-dimensional and highly-nonlinear functions. The difference between the first three methods is the setting of the regression parameter, which determines the method of calculating the weights implied by the unbiasedness condition: simple Kriging assumes a known constant trend; ordinary Kriging supposes an unknown, but predicted constant trend; universal Kriging presumes a low-order polynomial as the trend [21]. Regression Kriging is recommended for noisy data and applies an optimized regularization parameter to the correlation matrix [22]. GEK is usually preferred when the exact gradient information is given.

## B. Refinement strategies

For surrogate-based optimization, sample-point refinement should be done in each iteration step. The predicted value at the unobserved sample and the uncertainty of the prediction can be both used to refine the design space for the sake of facilitating global optimization. Therefore the possible improvement of the optimum under study at an unobserved location can be defined as,

$$I(\mathbf{x}) = \begin{cases} y_{\min} - \hat{y}(\mathbf{x}) & \hat{y} < y_{\min} \\ 0 & else \end{cases} \tag{1}$$

And the total expected improvement can be calculated with the following formula,

$$E[I(\mathbf{x})] = (y_{\min} - \hat{y})\Phi\left(\frac{y_{\min} - \hat{y}}{s}\right) + s\varphi\left(\frac{y_{\min} - \hat{y}}{s}\right) \tag{2}$$

where $y$ is the predicted value, $y_{\min}$ is the minimum in the database, $s$ is the Kriging error, $\Phi$ is the standard normal distribution function and $\varphi$ is the normal probability density function. By maximizing the total improvement, a new sample where a global optimum may exist is filled into the design space.

But in the case of sparse initial sampling, EI-based refinement may get trapped in a local optimum. So another refinement strategy by directly maximizing Kriging error is considered. This strategy helps improve the global search performance of the framework.

## V. Optimization strategies

This framework is based on an optimization framework [23] programmed in Python [24]. In the present surrogate-based framework, the optimization framework works as integrated module. The optimization methodologies in the framework consist of Simplex, Subplex, genetic algorithm and three gradient-based optimizers---conjugate gradient method, steepest decent method and variable metric method, in which only the genetic algorithm is a global optimizer.

For classical optimization, by directly using a high-fidelity solver, gradient-based optimizers are recommended because of their high efficiency. But the gradient-based optimizer is a local optimizer; in that case, a global optimum maybe omitted. Comparably, genetic algorithms are favored for global optimization, but the computational effort may be excessive. In view of that, surrogate-based optimization is adopted here instead of classical optimization, because it is quite cheap to acquire the results by evaluating the constructed surrogate model rather than the high-fidelity solver.

In the process of surrogate-based optimization, refinement strategies are used to resample the design space. In this paper, results for two refinement strategies are presented: optimize EI function and optimize the Kriging error. Both of these strategies are performed by using a genetic algorithm on the fitted surrogate model, because it is a global approximation of the cost function and cheap to evaluate.

## VI. Applications

### A. NACA 4-digit airfoil with 2 design parameters

To validate the optimization chain of the framework, an artificial objective function (3) is optimized for a 12% thick NACA 4-digit airfoil.

$$obj = C_D + 100*(C_L - 0.336)^2 + 100*(C_M + 0.0844)^2 \tag{3}$$

$C_D$, $C_L$ and $C_M$ are respectively the drag, lift and moment coefficient, and *obj* stands for the objective. The NACA 0012 airfoil is chosen as the baseline, and the separate effects of camber and the thickness distribution according to [19] are used in the parameterization to generate new geometries with the given design variables. For visualization of the process, two design variables are used for this problem: the position of the maximal camber and the maximal camber. The TAU deformation tool based on radial basis functions is applied to generate new grids providing the old grids and new geometries. Moreover, the TAU N-S solver with the Spalart-Allmaras turbulence model is used to compute the flow field at the design point Re=9.0e+6, Ma=0.8 and AoA=1.25$^{o}$. Ordinary Kriging is chosen to fit the surrogate model.

First the entire design space is “scanned” to plot the objective function and visualize the optima. As shown in Figure 3, this objective function has two optima, one local minimum and one global minimum respectively.

As shown in Table 1, different strategies are used to optimize the objective function. The results of simplex and gradient-based optimization depend on a start point in the vicinity of the global optimum can result in global results, and vice versa. By using genetic algorithm, the global optimum is always found with a large number of runs of the flow solver. Surrogate-based optimization with EI-based sample refinement can always obtain the global optimum except in the situations with rather bad initial sampling (e.g. 14 initial samples). Intuitive illustrations are shown in Figure 5(a) and 5(b). For the case with 14 initial samples in (a), although the 516 runs of the flow solver are larger, the optimization still trapped in the local minimum directly, because no more information about the global minimum is offered. For the case with 21 initial samples in (b), the main search direction is global, but it also makes effort to search locally. Comparing the number of the runs of the flow solver, the surrogate-based optimization gains more favor.

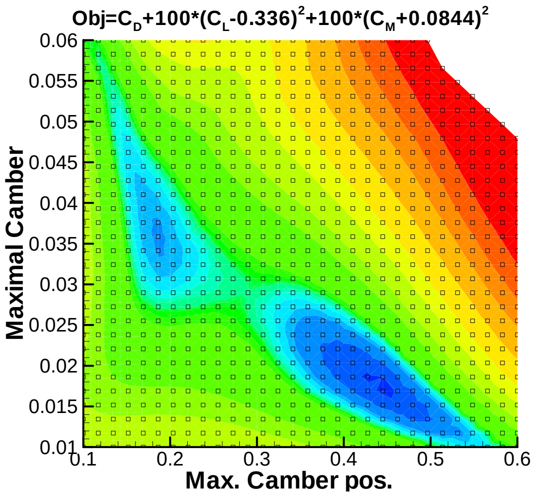



**Figure 3. Contour of the cost function from scanning the design space**

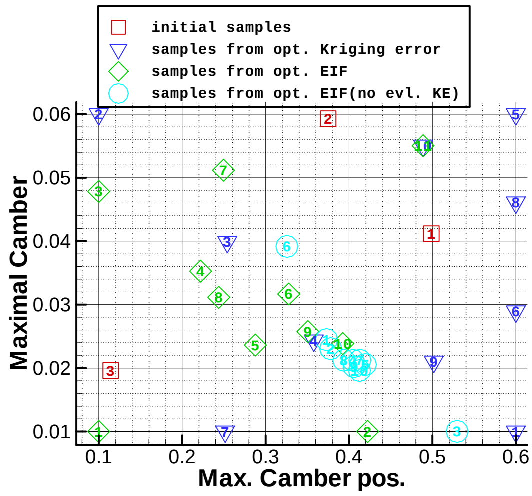
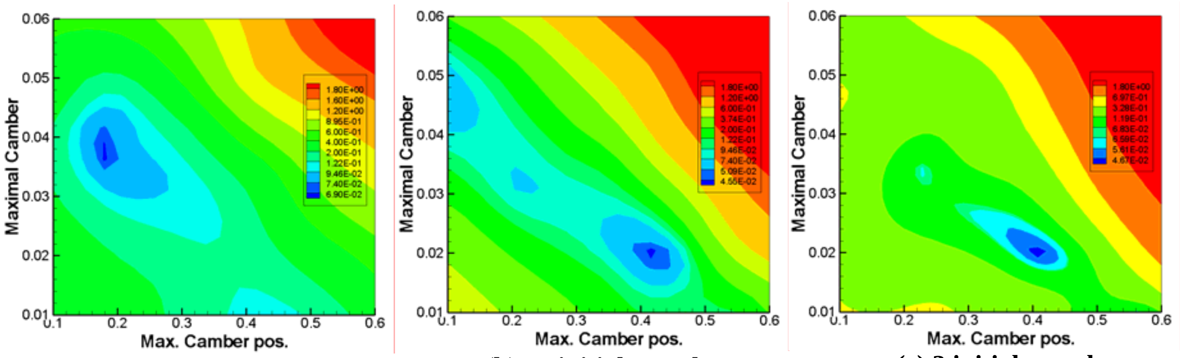



**Figure 4. New samples from two refinement strategies in optimization procedure**

**Table 1. Optimization of the artificial cost function for NACA 4-digital airfoil**

| Strategy | Initial samples | Start | TAU runs | Results | |
|---|---|---|---|---|---|
| | | | | D. V. | Cost value |
| **Gradient** | × | [0.1,0.03] | 238 | [0.418516, 0.018175] | 0.042178 |
| **Simplex** | × | [0.1,0.03] | 69 | [0.209570, 0.032490] | 0.061397 |
| | × | [0.3,0.025] | 138 | [0.419624, 0.018131] | 0.042173 |
| **Genetic Algorithm** | × | [0.3,0.025] | 594 | [0.419621, 0.018131] | 0.042173 |
| **EI** | 8(LHS) | × | 295 | [0.411680, 0.019166] | 0.042997 |
| | 11(LHS) | × | 56 | [0.417681, 0.019561] | 0.042997 |
| | 14(LHS) | × | 516 | [0.182645, 0.036848] | 0.067040 |
| | 18(LHS) | × | 95 | [0.418833, 0.019414] | 0.042973 |
| | 21(LHS) | × | 24 | [0.432195, 0.019094] | 0.041977 |
| **EI(20)+Opt. KE(10)+Grad. Opt.** | 3(LHS) | × | 51 | [0.413275, 0.018615] | 0.042366 |

In order to avoid the risk of refining the surrogate model around a local optimum because of the bad sampling (including sparse sampling and one-sided sampling), a hybrid adaptive refinement strategy based on EI function and KE is employed and combined with a gradient-based optimization which starts from the optimum from surrogate-based optimization. Thus, after refinement of the surrogate model, in which procedure a global search has been done over the entire design space, a local search can converge very fast to the global optimum. In the test case using the hybrid strategy with only three initial samples shown in table 1, surrogate-based optimization just needs 20 runs of the flow solver, in which KE-based refinement is switched on only within the first 10 iteration steps, and then gradient-based optimization is started. Finally after a total of 51 high-fidelity flow computations, a global optimum is captured. As shown in Figure 5(c), large effort has been paid for searching globally.




**(a) 14 initial samples (EIF refinement)** **(b) 21 initial samples (EIF refinement)** **(c) 3 initial samples (hybrid refinement)**

**Figure 5. Contour of cost function interpolating on the finally gained surrogate model with different strategies**

The samples from two refinement strategies generated in each iteration step are plotted in Figure 4. Three red squares stand for the initial samples. 10 blue down-triangles are samples from KE-based refinement, most of which are located on the boundary; it indicates that this strategy did help search globally. Diamonds and circles represent samples from EI-based refinement, in which green diamonds are samples within the first 10 iterations. It shows that EI-based refinement at first tries to refine the design space globally (diamonds), then locally (circles).

## B. NLF0416 airfoil with 10 design parameters

Optimization of the drag for an NLF0416 airfoil with 10 design parameters is performed. There are 5 design variables on the upper and lower surface respectively. They are the bumps of the control points for the geometry, with the x-positions 0.1, 0.2, 0.4, 0.6 and 0.8. A N-S flow solver combined with a transition prediction module and the Spalart-Allmaras turbulence model is run at the design point Re=2.0e+6, Ma=0.1 and a targeted lift coefficient $C_L$=0.72. The range of each design variable is defined as [-0.01, 0.01]. Regression Kriging with constant regularization is used to construct the surrogate model.

**Table 2. Optimization of the drag for NLF 0416 airfoil**

| Profile | $C_L$ | $C_D$ (0.0001) | $C_{Dv}$ (0.0001) | $C_{Dp}$ (0.0001) | Trans. Point (x/C) | TAU Comp. (runs) |
|---|---|---|---|---|---|---|
| **Baseline** | 0.719253 | 82.30 | 53.58 | 28.72 | 0.333021 | × |
| **Subplex** | 0.720562 | 79.64 | 52.06 | 27.58 | 0.344047 | 190 |
| **EI** | 0.719192 | 79.74 | 52.30 | 27.44 | 0.355069 | 69 |
| **EI+Simplex Opt.** | 0.719990 | 79.56 | 52.13 | 27.43 | 0.355069 | 81 |
| **EI+Simplex Opt. (new range)** | 0.720659 | 75.03 | 48.24 | 26.79 | 0.486853 | 71 |

10 initial samples from LHS are used as a DoE plan. Surrogate-based optimization is run with EI-based refinement. Then optimization using a local optimizer Simplex is started from the optimum from surrogate-based optimization. In order to compare the accuracy and efficiency of this framework, classical optimization using Subplex is run with the start from the baseline. The results are shown in Table 2. The strategy, combining surrogate-based optimization and classical optimization, shows best accuracy with just 12 additional flow computations in classical optimization using Simplex.

The geometries of the profiles are shown in Figure 6. The corresponding pressure distributions are presented in Figure 7. Surrogate-based optimization with EI refinement and combined with classical optimization both acquire better pressure distributions that have a more flat top. But considering the small improvement in terms of drag, the optimum found isn't actually the perfect result. It seems that the transition point is restricted. In the author's opinion, this is due to the narrow range of the design variables. Therefore, the case is performed again with a larger range of the design variables (new ranges are shown in Table 3). From the results in Table 2, the drag coefficient decreases nearly 7.3 drag counts, and the number of the runs of the flow solver is only 71, which, compared with classical optimization using Subplex, is quite lower. The efficiency of the optimization is satisfying.

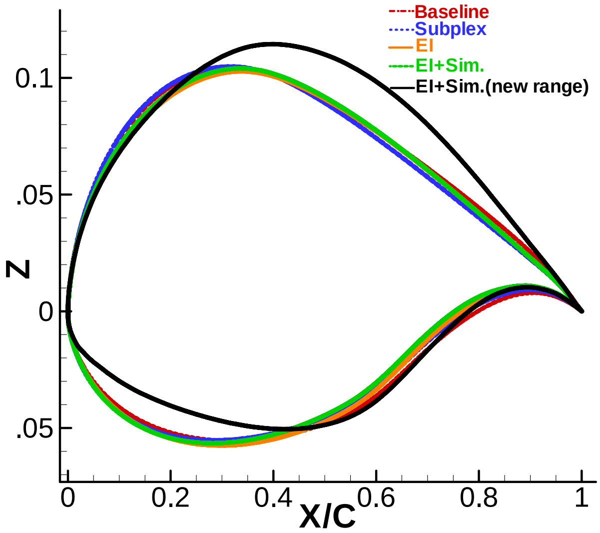



**Figure 6. Geometries of the profiles**

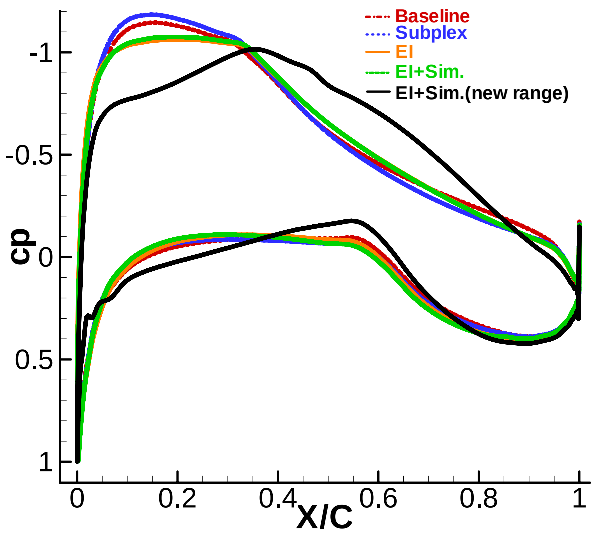



**Figure 7. Pressure distributions of the profiles**

**Table 3. New range of the design variables for NLF 0416 airfoil**

| Design Variables | DV1 | DV2 | DV3 | DV4 | DV5 | DV6 | DV7 | DV8 | DV9 | DV10 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Min.** | -0.01 | -0.02 | -0.04 | -0.02 | -0.01 | -0.01 | -0.03 | -0.06 | -0.04 | -0.02 |
| **Max.** | 0.01 | 0.05 | 0.09 | 0.07 | 0.06 | 0.01 | 0.03 | 0.05 | 0.03 | 0.02 |

## VII. Conclusions

Due to the requirement of a practical, efficient tool for global optimization, a framework combining different CFD solvers, DoE methods, optimization algorithms and various surrogate modeling methodologies with sample refinement strategies is under development. Moreover the strategy of performing a local optimizer starting from the optimum from surrogate-based optimization is studied aiming to improve the efficiency and accuracy of the framework. This hybrid strategy is applied to the test cases of a NACA 4-digit airfoil with 2 design variables and an NFL0416 airfoil with 10 design variables. The results confirm that the present framework with the hybrid strategy is much more efficient than classical optimization for multi-dimension and multi-optima problems with acceptable accuracy.

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