COMBINING ADJOINT-BASED AND SURROGATE-BASED OPTIMIZATIONS FOR BENCHMARK AERODYNAMIC DESIGN PROBLEMS

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Abstract

In recent years, surrogate-based modeling and optimization have received much attention in the area of aerodynamic design optimization (ADO). However, for high-dimensional problems with large number of design variables, surrogate-based optimization (SBO) is suffering from the prohibitive computational cost associated with evaluating a large number of sample points by high-fidelity and expensive computational fluid dynamics (CFD) simulations. In this paper, we propose to use gradient-enhanced kriging (GEK) to combine the adjoint-based and surrogate-based optimizations, to greatly improve the efficiency of global optimization. The GEK model is integrated to a surrogate-based optimizer and demonstrated for Benchmark Case 1, Case 2 and Case 4 developed by the AIAA Applied Aerodynamics Discussion Group (ADODG), with the number of design variables in the range from 18 to 42. It is observed that, GEK model is much more efficient than the traditional kriging model, indicating that the proposed method has great potential for breaking or at least ameliorating the "curse of dimensionality" for higher-dimensional engineering design problems.

1 Introduction

Over past few decades, CFD–based aerodynamic design optimization (ADO) has been highly developed and widely applied in the area of aircraft design. The CFD-based ADO methods can be classified into three categories: direct gradient-based optimization algorithm, derivative-free optimization algorithm and surrogate-based optimization (SBO). Among them, the gradient-based optimization with gradients calculated by using an adjoint approach has proved effective and got popularity for aerodynamic shape optimization via high-fidelity CFD methods [1]. It can deal with the optimization problems with 100-1000 design variables [2]. However, the drawback of this method is that it can be sensitive to the initial design and can be trapped into a local minimum. In contrast, the derivative-free methods, e.g. Evolutional Algorithms (EA), is capable of finding global optimum, whereas the computational cost can be prohibitive due to the evaluation of a large number of high-fidelity CFD simulations. Typically, at least thousands of CFD simulations are required when using an EA method for aerodynamic shape optimization. The third method, SBO, represents a type of algorithm that makes use of surrogate models to approximate to the expensive objective and constraint functions, throughout the design space or within specific region, driving the addition and evaluation of new sample point(s) towards global or local optimum(s)[3][4]. It has been proved very effective for ADO problems. However, when dealing with complex aircraft configuration parameterized by many design variables, a large number of expensive-to-evaluate samples will be needed to construct a reasonably accurate surrogate model, which inspires the use of cheap-to-evaluate auxiliary information, such as lower-fidelity data or gradient information, to improve the accuracy of building surrogate models towards the reduction of the number of high-fidelity CFD simulation.

In this paper, we propose to combine adjoint-based and surrogate-based optimizations through GEK model. The cheap gradient information is obtained by using an adjoint method. Then the gradient information is directly included in the kriging equations system by augmenting the weighted sum of the gradients to the weighted sum of the observed functional values. This way of exploiting the benefit of cheap gradient information on the constructing of a kriging model is called direct GEK [5][6][7]. The GEK model is integrated to a surrogate-based optimizer and demonstrated for three benchmark cases defined by the AIAA aerodynamic design optimization discussion group (ADODG). The first two cases are the drag minimizations of NACA 0012 airfoil and RAE 2822 airfoil in transonic flow, using Euler and Reynolds-averaged Navier-Stokes (RANS) flow solvers, respectively, with the number of design variables in the range from 18 to 42. To fully explore the proposed method's capability for more complex aerodynamic shape optimization case, the lift-constrained drag minimization of the ADODG Common Research Model (CRM) wing using a RANS solver is also formulated, with 38 design variables.

The remainder of the paper is organized as following: section 2 and 3 review the theory and algorithms of adjoint method and GEK model; section 4 introduces the in-house SBO toolbox SurroOpt and the open source CFD solver SU2; section 5 presents examples to compare the performance of GEK model and kriging model when used for aerodynamic design optimizations. The last section gives conclusions and outlook.

2 Overview of Adjoint Method

Here we only give a brief overview about the adjoint method. The readers are referred to literatures such as [8] for more details about the formulation.

In an aerodynamic design such as airfoil or wing design, the aerodynamic shape can be parameterized by a set of design variables $\mathbf{x}=(x_i), i=1,..,n$. The cost function (e.g. drag coefficient) is a function of $\mathbf{x}$ and flowfield variable $\mathbf{W}$:

$$I = I(\mathbf{W},\mathbf{x}) \ , \tag{1}$$

and a change in $\mathbf{x}$ results in the change

$$\delta I = \frac{\partial I^T}{\partial \mathbf{W}}\delta \mathbf{W} + \frac{\partial I^T}{\partial \mathbf{x}}\delta \mathbf{x} \ . \tag{2}$$

Suppose that the governing equations of the flowfield can be written as

$$\mathfrak{R}(\mathbf{W},\mathbf{x}) = 0 \ . \tag{3}$$

Then $\delta\mathbf{W}$ can be determined from

$$\delta\mathfrak{R} = \frac{\partial \mathfrak{R}}{\partial \mathbf{W}}\delta \mathbf{W} + \frac{\partial \mathfrak{R}}{\partial \mathbf{x}}\delta \mathbf{x} = 0 \ . \tag{4}$$

After introducing a Lagrange multiplier Ψ , we have

$$\begin{aligned}\delta I &= \left[\frac{\partial I}{\partial \mathbf{W}}\right]^T \delta\mathbf{W} + \left[\frac{\partial I}{\partial \mathbf{x}}\right]^T \delta\mathbf{x} - \Psi^T\left(\frac{\partial \mathfrak{R}}{\partial \mathbf{W}}\delta\mathbf{W} + \frac{\partial \mathfrak{R}}{\partial \mathbf{x}}\delta\mathbf{x}\right) \\ &= \left(\left[\frac{\partial I}{\partial \mathbf{W}}\right]^T - \Psi^T\frac{\partial \mathfrak{R}}{\partial \mathbf{W}}\right)\delta\mathbf{W} + \left(\left[\frac{\partial I}{\partial \mathbf{x}}\right]^T - \Psi^T\frac{\partial \mathfrak{R}}{\partial \mathbf{x}}\right)\delta\mathbf{x}\end{aligned} \ . \tag{5}$$

Choosing Ψ to satisfy the adjoint equation

$$\psi[\frac{\partial \mathfrak{R}}{\partial \mathbf{W}}]^T = \frac{\partial I}{\partial \mathbf{W}} \ . \tag{6}$$

Then the first term of equation (5) can be eliminated, and the gradient can be found by

$$\mathbf{G}(\mathbf{x}) = \frac{\partial I}{\partial \mathbf{x}} = [\frac{\partial I}{\partial \mathbf{x}}]^T - \psi^T\frac{\partial \mathfrak{R}}{\partial \mathbf{x}} \ . \tag{7}$$

We can see that the computational cost of evaluating the gradients of I is nearly independent of number of design variables.

Once the cheap gradient is obtained, it can used to improve the accuracy of a surrogate model, such as kriging. The details of constructing such a kriging model are given in next section.

3 Gradient-Enhanced Kriging Formulation

3.1 GEK Predictor and Its MSE

For an m- dimensional problem, suppose we are concerned with the prediction of an expensive-to-evaluate high-fidelity aerodynamic function $y:\mathbb{R}^m \to \mathbb{R}$. Firstly, we choose n sample sites by using the method of design of experiments (DoE) and then run CFD and adjoint codes to get the responses of the aerodynamic function as well as its gradients with respect to the design variables. Then the sampled dataset $(\mathbf{S}, \mathbf{y}_S)$ are formed as

$$\begin{aligned}&\mathbf{S} = [\mathbf{x}^{(1)},\cdots,\mathbf{x}^{(n)},\cdots,\mathbf{x}^{(n)},\cdots,\mathbf{x}^{(n)}]^{\mathrm{T}} \in \mathbb{R}^{(n+nm)\times m}\\ &\mathbf{y}_S = [y^{(1)},\cdots,y^{(n)},\cdots,\frac{\partial y^{(n)}}{\partial x_1},\cdots,\frac{\partial y^{(n)}}{\partial x_m}]^{\mathrm{T}} \in \mathbb{R}^{n+nm}\end{aligned}. \tag{8}$$

The prediction of a GEK model at an untried $\mathbf{x}$ is formally defined by augmenting the weighted sum of the observed gradients to the weighted sum of the observed function values as

$$\hat{y}(\mathbf{x}) = \sum_{i=1}^{n} w^{(i)} y^{(i)} + \sum_{j=1}^{m}\sum_{i=1}^{n} \lambda_j^{(i)} \frac{\partial y^{(i)}}{\partial x_j}, \tag{9}$$

where $w^{(i)}$ represents the weight coefficient for the observed values of aerodynamic function at i-th sampling site, and $\lambda_j^{(i)}$ denotes the weight coefficient for an observed partial derivative of the aerodynamics function, taken at i-th sampling site and with respect to j-th design variable. There are $n(1+m)$ weight coefficients in total, whose optimal values are to be obtained by using a Lagrange multiplier method.

As for a kriging model, the GEK predictor can be proven to be of the form

$$\hat{y}(\mathbf{x}) = \beta_0 + \bar{\mathbf{r}}^{\mathrm{T}}(\mathbf{x})\underbrace{\bar{\mathbf{R}}^{-1}(\mathbf{y}_S - \beta_0\bar{\mathbf{F}})}_{\mathbf{V}_{GEK}}, \tag{10}$$

where

$$\begin{aligned}&\beta_0 = \left(\bar{\mathbf{F}}^{\mathrm{T}}\bar{\mathbf{R}}^{-1}\bar{\mathbf{F}}\right)^{-1}\bar{\mathbf{F}}^{\mathrm{T}}\bar{\mathbf{R}}^{-1}\mathbf{y}_S\\ &\bar{\mathbf{F}} = (\underbrace{1,..,1}_{n},\underbrace{0,..,0}_{nm})^{\mathrm{T}} \in \mathbb{R}^{n+nm}\end{aligned}, \tag{11}$$

and $\bar{\mathbf{R}}$ and $\bar{\mathbf{r}}$ are the augmented correlation matrix and correlation vector, respectively. They are of the form

$$\begin{aligned}&\bar{\mathbf{R}} = \begin{bmatrix}\mathbf{R} & \partial\mathbf{R}\\ \partial\mathbf{R}^{\mathrm{T}} & \partial^2\mathbf{R}\end{bmatrix} \in \mathbb{R}^{(n+nm)\times(n+nm)}\\ &\bar{\mathbf{r}} = \begin{bmatrix}\mathbf{r}\\ \partial\mathbf{r}\end{bmatrix} \in \mathbb{R}^{n+nm}\end{aligned}. \tag{12}$$

The mean-squared error (MSE) of the GEK prediction, as a kind of uncertainty at any untried $\mathbf{x}$ can be proven to be

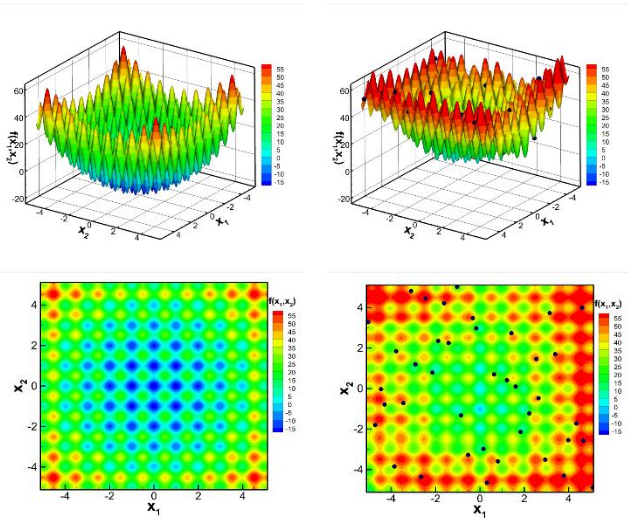
$$\begin{aligned}&\mathrm{MSE}\{\hat{y}(\mathbf{x})\} = s^2(\mathbf{x})\\ &= \sigma^2\{1.0 - \bar{\mathbf{r}}^{\mathrm{T}}\bar{\mathbf{R}}^{-1}\bar{\mathbf{r}} + (1-\bar{\mathbf{F}}\bar{\mathbf{R}}^{-1}\bar{\mathbf{r}})^2/(\bar{\mathbf{F}}^{\mathrm{T}}\bar{\mathbf{R}}^{-1}\bar{\mathbf{F}})\}\end{aligned}. \tag{13}$$

3.2 Validation of GEK Model

In this subsection, the following two-dimensional test function is used to explain the procedure of building a GEK model and to verify its correctness:

$$\begin{aligned}&f(x) = \sum_{i=1}^{2}\left(x_i^2 - 10\cos(2\pi x_i)\right)\\ &x_1, x_2 = [-5.12, 5.12]\end{aligned}. \tag{14}$$

Forty sampling sites are chosen by Latin hypercube sampling (LHS) [9] method and the functional response values as well as corresponding gradients are obtained analytically. The results are shown in Fig 1. The GEK model is compared with the exact function by plotting both the contour and isocline, which validates the correctness of the proposed GEK model.



(a) Exact function **(b) GEK**

Fig 1. Validation of GEK model for a 2-D test function

4 Methodology

4.1 SBO Framework

The GEK model has been integrated into an in-house optimization code called "SurroOpt" [10]-[15]. SurroOpt is a state-of-the-art, surrogate-based optimization code developed for academic research and engineering designs driven by expensive numerical simulations. It can be used to efficiently solve arbitrary single and multi-objective (Pareto front), unconstrained and constrained optimization problems.

In SurroOpt, building GEK models and solving sub-optimization problems corresponding to the infill-sampling criteria are taken as an optimization mechanism, whose role is the same as any of the conventional gradient-based methods or heuristic optimization algorithms. This new optimization mechanism leads to the automatic clustering of sample points near the optimum and the GEK models are not necessarily accurate throughout the whole design space. As a result, the selection of initial samples and the approximation accuracy of the initial GEK models have less effect on the final optimum. The framework of proposed GEK-based method is shown in Fig 2.

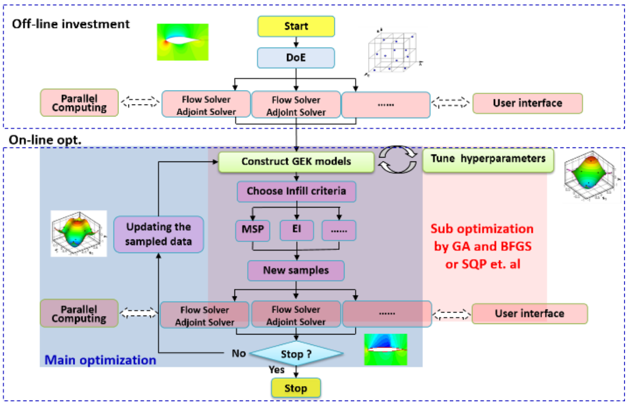


Fig 2. **Framework of proposed GEK-based method that combines adjoint gradients with surrogate-based optimization [10]**

4.2 SU2 software suite

In this paper, the Stanford University SU2 code [16] is applied for the geometric parameterization, mesh deformation, as well as flow solution and adjoint gradient evaluation based on the Euler and RANS equations.

SU2 is an open-source computational analysis and design package that has been developed to solve multi-physics analysis and optimization tasks using unstructured mesh topologies. It provides a number of geometry parameterization techniques. In this paper, a free-form deformation (FFD) strategy is adopted to parameterize the airfoil and wing geometry. In this method, the object (airfoil and wing in this paper) is encapsulated by an initial FFD box which is parameterized as a Bézier solid. A set of control points on the surface of the box are defined as design variables, and the geometry of the object inside the box can be deformed by modifying these control points. After perturbing the geometry, an approach based on the linear elasticity equations [17] is used to propagate the deformation to the surrounding volume mesh.

Both continuous and discrete adjoint approaches for the Euler and RANS equations are available in SU2, while the discrete adjoint method is applied in this paper to efficiently compute the gradients required by building the GEK model.

5 Examples

5.1 Benchmark Case I: Drag Minimization of NACA 0012 Airfoil in Transonic Inviscid Flow

The optimization problem of this work is the drag minimization of a modified NACA 0012 airfoil at a free stream Mach number of 0.85 and at a zero angle of attack, subject to a full thickness constraint. In summary, the mathematical model is of the form

$$\begin{aligned} &\text{minimize} && c_d \\ &\text{with respect to} && c_l = 0.0 \\ & && y \geq y_{\text{baseline}} \quad \forall x \in [0,1]. \end{aligned} \qquad (15)$$

An O-type grid for inviscid flow simulation is applied to this case as shown in Fig 3. Furthermore, since the airfoil is symmetrical and the angle of attack is fixed at zero, only the half-plane is considered to avoid the difficulties due to non-symmetrical solutions. A series of grids are generated using a hyperbolic mesh generator to perform a grid convergence study as shown in Tab 1. The middle grid size is used for optimization, since the difference between the medium-size and large-size grids is less than 0.1 counts (1 drag count is $\Delta c_d = 10^{-4}$)

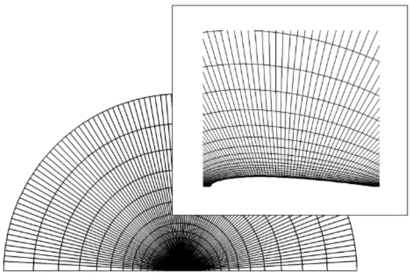


Fig 3. The half-plane of O-type mesh used in case 1

Tab 1. Grid convergence study for NACA 0012 airfoil

Grid size	NACA 0012 (c_d counts)
L1:126×126	470.036
L2:256×256	470.804
L3:512×512	470.872

Two FFD frames are used in this work. The first is a coarser FFD volume with 48 control points arranged in a 15×2 pattern, corresponding to 19 design variables in total, as shown in Fig 4. The second FFD is based on a finer pattern (26×2), with 42 design variables chosen to examine the performance of GEK in the problems with a middle size of design variables. It is worth noting that the method considers both x and y coordinates of specific control points near the leading and trailing edge.

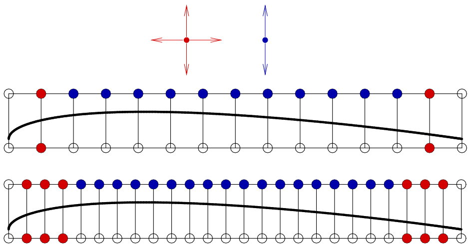


Fig 4. Sketch of two kinds of FFD frames (the red control points can move in both x and y direction, while the blue points can only move in y direction and the others are fixed.

To validate the accuracy of the gradient information obtained by the discrete adjoint formulation, a comparison was made between the discrete adjoint approach and finite-difference approach. The step size of the FFD deformation for both methods is 0.001c. The results are shown in Fig 5. And one can see that the gradients obtained by using the adjoint method agree well with the results from the finite-difference method, indicating that the adjoint solver has a reasonable accuracy in calculating gradients.

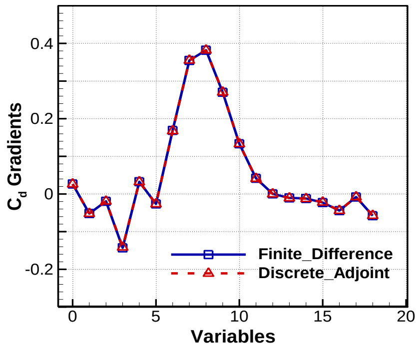
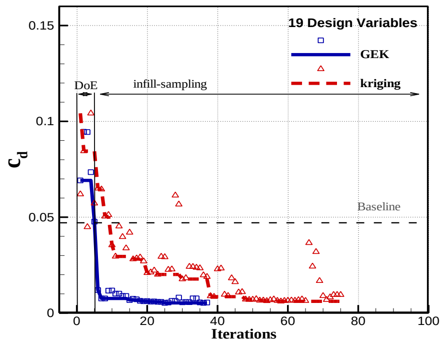


Fig 5. Comparison of adjoint method and finite difference method for the gradients of drag w.r.t. the design variables

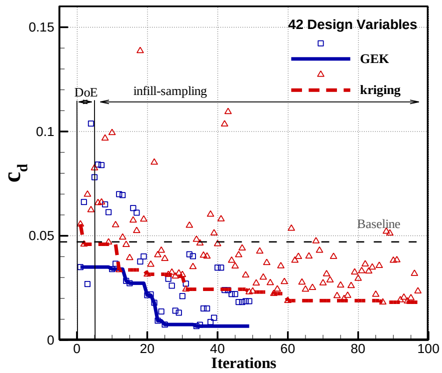
In this benchmark, 5 initial sample points are chosen by LHS method. Note that EI+MSP (maximizing the expected improvement and minimizing the surrogate prediction) infill-sampling criterion is used to choose new samples and drive the optimization towards optimum.

Fig 6 shows the convergence histories of optimizations based on GEK or kriging model. When using a GEK, the drag coefficient is reduced to 56.11 counts (1 drag count is $\Delta c_d = 10^{-4}$) with 19 design variables, comparing with 61.06 counts for kriging model. When the number of design variable is increased to 42, we found that the cost of building a GEK model dramatically increased, which is caused by the huge correlation matrix of a GEK. The current optimal value for this setting is 67.05 counts, which is higher than using 19 design variables (56.11 counts). The possible reason is the ill-conditioning of correlation matrix due to poorly spaced samples, which is a major challenge necessary for robust and efficient GEK emulators. The situation for the kriging model is much worse, with a value of 181.42 counts after infilling nearly 80 samples. Some further improvement is likely possible, but it will need a large number of sample-point evaluations. This is consistent with our experience that one will need a large number of samples to build a sufficiently accurate kriging model for high-dimensional problems, which is also known as the “curse of dimensionality”.

We can see from both cases that the GEK-based method is much more efficient than the kriging-based method, especially for the problems with a medium size of design variables.



(a) 19 design variables



(b) 42 design variables

Fig 6. Convergence history of optimization for ADODG case 1

The surface pressure distributions of NACA 0012 and optimal airfoils are exhibited in Fig 7. The leading edge has become extremely blunt in all cases. This is the expected optimal result for this problem, though this shape would have poor viscous performance. By the final design, the containment constraint is satisfied everywhere.

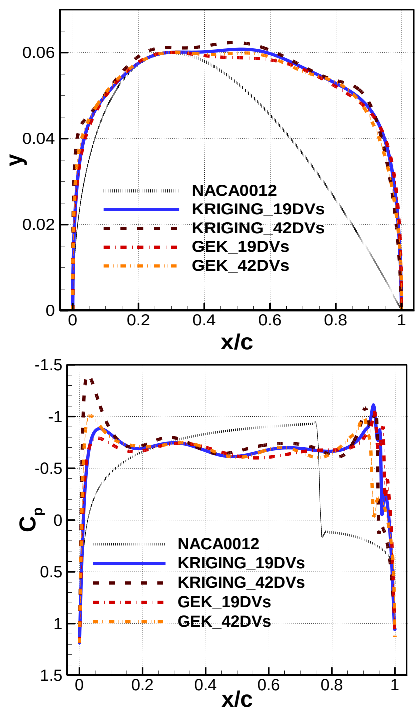


Fig 7. Shapes and pressure coefficient distributions for baseline and optimized airfoils

Tab 2. Drag coefficients (counts) of baseline NACA 0012 and optimal airfoils

	GEK	Kriging
Baseline	470.80	
19 DVs	56.11	61.06
42 DVs	67.05	181.42

5.2 Benchmark Case II: Drag Minimization of RAE 2822 Airfoil in Transonic Viscous Flow

Case II revisits transonic airfoil design (Mach 0.734), but this time with more realistic design constraints. The objective is again to reduce the drag, while constraints are imposed on lift, pitching moment (which is initially violated) and the area:

$$\begin{aligned} &\text{minimize} && c_d \\ &\text{with respect to} && c_l = 0.824 \\ & && c_m \geq -0.092 \\ & && \text{Area} \geq \text{Area}_{initial} \approx 0.07787c^2 \end{aligned} \quad . \qquad (16)$$

A hybrid mesh is adopted, as show in Fig 8. the grid convergence study is conducted and the results are shown in Fig 9. The medium-size grid is used for optimization.

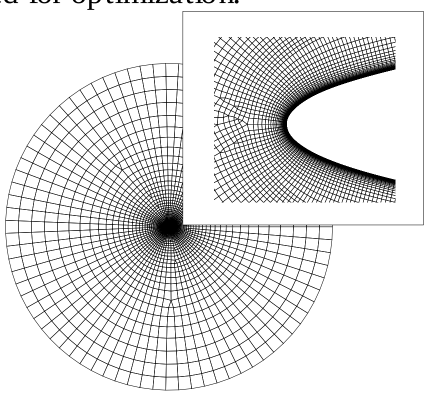
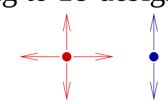


Fig 8. The hybrid mesh used in case 2

Tab 3. Grid convergence study for RAE 2822 airfoil

Grid size	c_l	c_d (counts)
30079	0.824	199.0
41573	0.824	196.8
53510	0.824	197.4

The definition of FFD frame is shown in Fig 9, corresponding to 18 design variables in total.



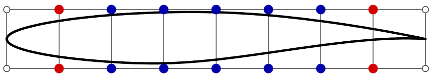


Fig 9. The definition of FFD frame used in ADODG case 2

In this benchmark, 6 initial sample points are chosen by LHS method and the EI infill-sampling criterion is applied. The convergence history of optimization is shown in Fig 10, which indicates GEK can significantly improve the efficiency of optimization, when compared with kriging, although the optimum obtained from kriging is slightly better than that of GEK.

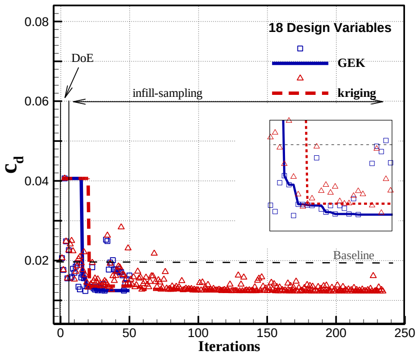


Fig 10. Convergence history of ADODG benchmark case 2

Tab 4. Performance convergence of baseline RAE2822 airfoil and optimal airfoils

	c_d	c_l	c_m	*Area*
Baseline	196.8	0.824	-0.095	0.07784
GEK	124.7	0.824	-0.083	0.07784
Kriging	123.0	0.824	-0.089	0.07784

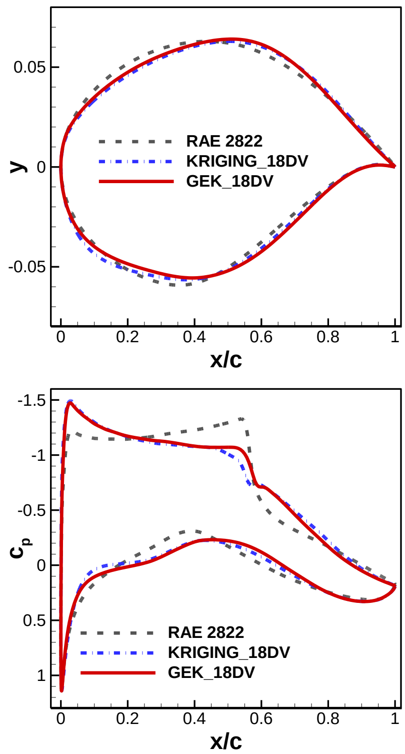


Fig 11. Shapes and pressure coefficient distributions for baseline and optimized airfoils

From Fig 11, one can see that the shock is nearly eliminated for both optimal airfoils, indicating the multimodality of this optimization case.

5.3 Benchmark Case Ⅳ: Drag Minimization of CRM Wing in Transonic Viscous Flow

The final case is a wing design optimization problem at Mach 0.85. The objective is to reduce the drag, subject to a lift constraint and a pitching moment constraint, which is initially violated. The baseline geometry is the Common Research Model (CRM) wing. The planform is fixed, while variation in the vertical direction is permitted, including airfoil design and sectional twist. The wing is required to maintain its initial volume and also to maintain at least 25% of its original local thickness everywhere. The full optimization problem is

$$\begin{aligned} &\text{minimize} && C_D \\ &\text{with respect to} && C_L = 0.5 \\ & && C_M \geq -0.17 \\ & && \text{Volume} \geq \text{Volume}_{initial} \\ & && \text{Thickness} \geq 0.25\text{Thickness}_{initial} \\ & && \Delta Z_{\text{TE}} = 0 \\ & && \Delta Z_{\text{LE,root}} = 0 \end{aligned} \qquad (17)$$

Fig 12 shows the structured mesh used in this test case. The parameters in this case are the vertical displacements of control points located on the FFD control box, corresponding to 38 design variables. The FFD volume definition is shown in Fig 13.

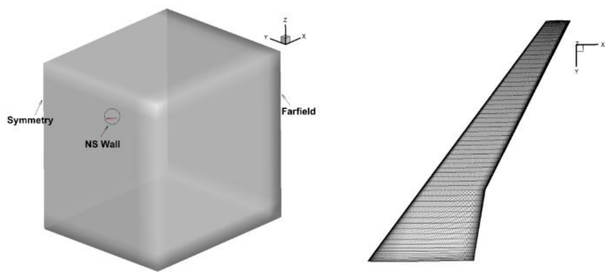


Fig 12. The structured mesh used in ADODG case 4

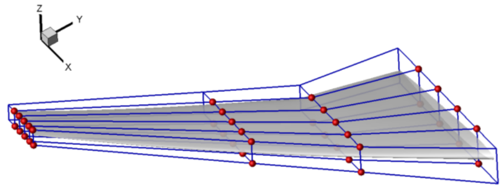


Fig 13. CRM wing FFD control box (in blue) and selected control points (in red) as design variables

A comparison of gradients was made between the discrete adjoint approach and finite different approach, as shown in Fig 14. The results verify the accuracy of the gradients obtained from the discrete adjoint method.

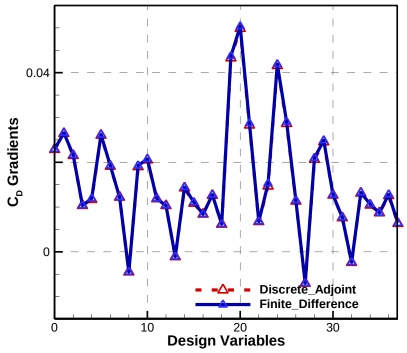


Fig 14. Comparison of adjoint method and finite difference method for the gradients of drag w.r.t. the design variables

16 initial sample points are chosen by LHS method and the EI infill-sampling criterion is used to repetitively select new sample points. Fig 15 shows the convergence history of optimization. One can see that the GEK-based method outperforms the kriging-based method in terms of the efficiency and the final optimum, with the drag being reduced by 8.9 counts and 6.5 counts respectively.

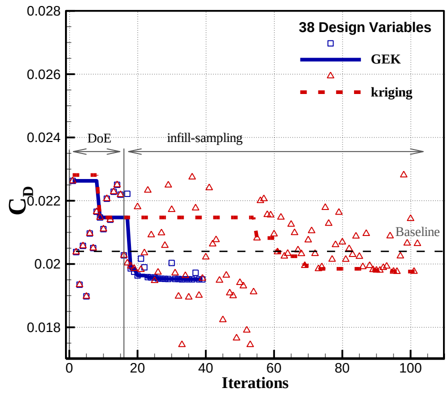
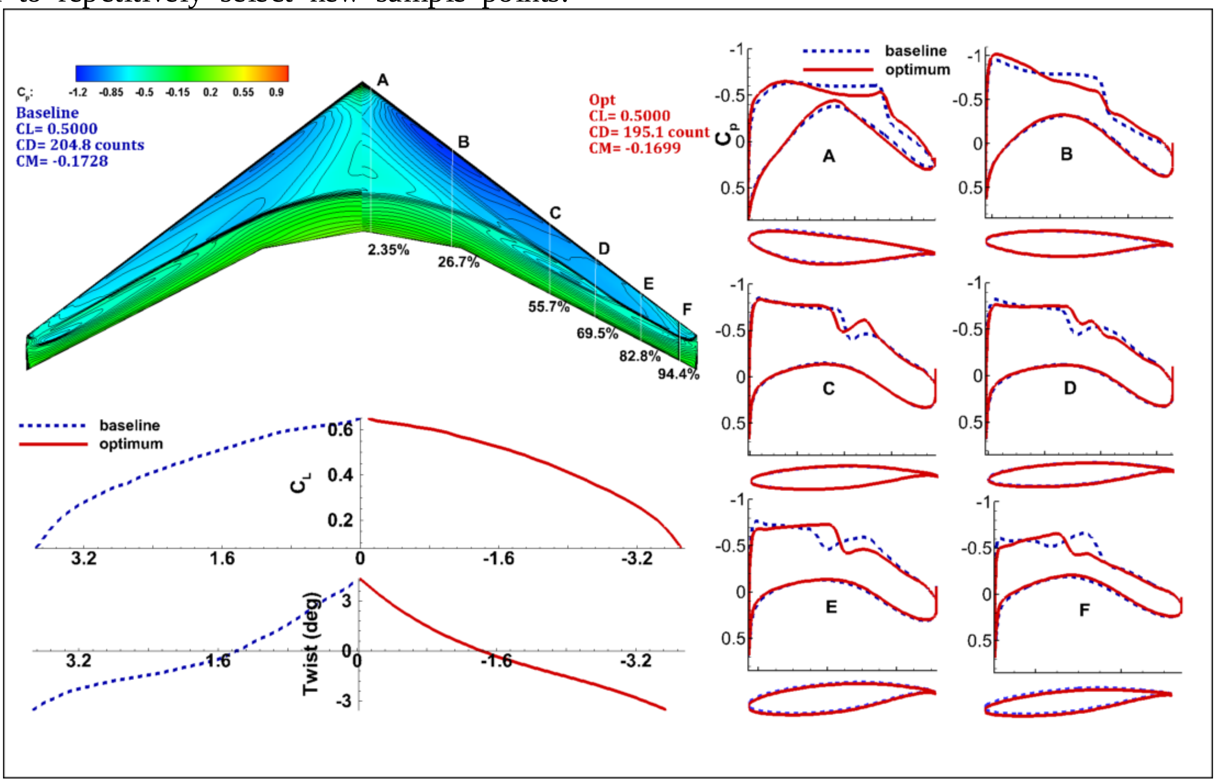


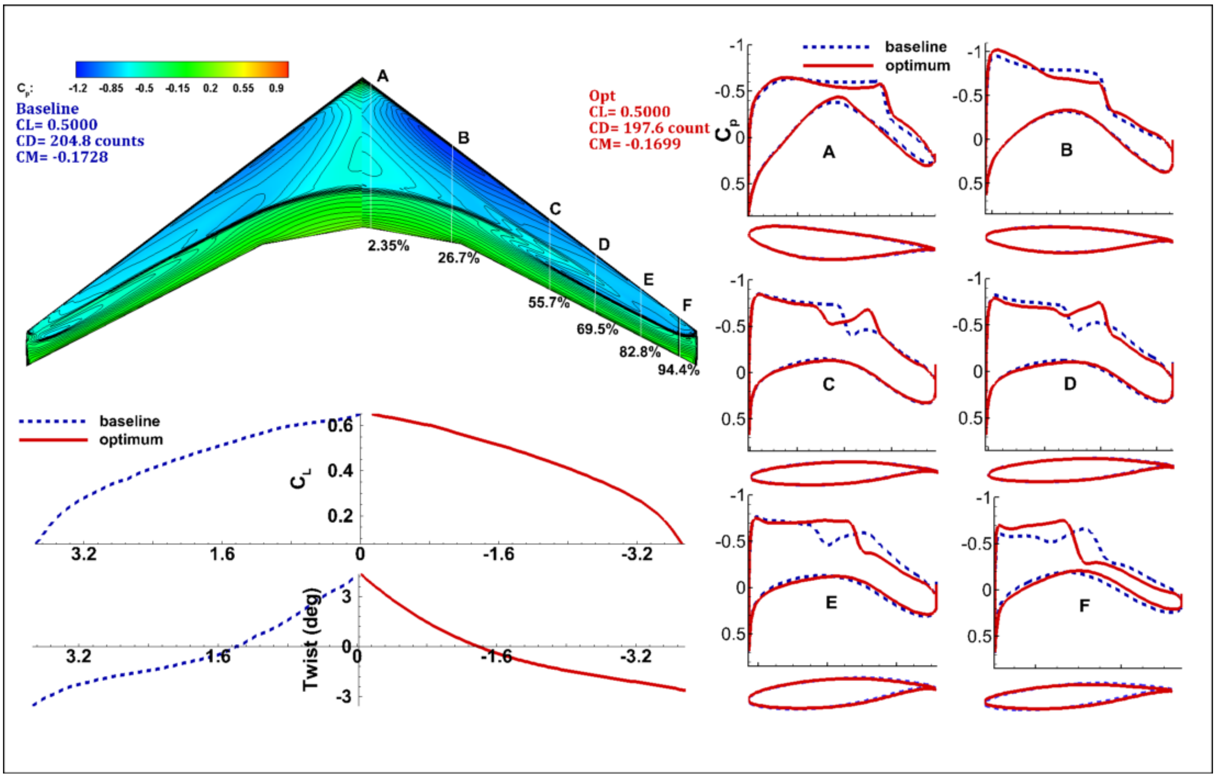
Fig 15. Convergence history of ADODG benchmark case 4

Tab 5. Force coefficients and volume of CRM wing and optimal wings

	C_L	C_D (counts)		C_M	Volume
		$C_{D,p}$	$C_{D,f}$		
Baseline	0.500	143.8	61.1	-0.1728	0.2583
GEK	0.500	133.9	61.3	-0.1699	0.2584
Kriging	0.500	136.4	61.2	-0.1699	0.2585



(a) The optimal wing by GEK-based optimization



(b) The optimal wing by kriging-based optimization

Fig 16. Comparison between the baseline and the optimized wings

Fig 16 shows the comparison between the baseline and the optimized wings. In these figures, the results of baseline wing are shown in blue and the optimized wing results are shown in red. At the optimum, the lift coefficient target is met and the pitching moment is reduced to the lowest allowed value. The baseline wing exhibits a strong shock, while the two optimized wings from GEK-base and kriging-based methods both have a lower pressure drag associated to a weaker shock wave at the inboard sections. However, there still exists a relative strong shock wave at the outboard sections for both optimized wings. Existing literature indicates that, to achieve a strong reduction of the pressure drag, the optimization algorithm has to make at the same time the inboard sections very thick and the outboard sections very thin [18]. This mechanism is not captured in our work. The possible reason could be the lack of the design variables. In the future, a larger number of design variables should be adopted to have a finer control over the geometry, especially the leading edge of wing.

6 Conclusions and Outlook

In this paper, we build a GEK model to combining the adjoint gradients with surrogate-based optimizations. It is then integrated to a surrogate-based optimizer and demonstrated for benchmark cases 1, case 2 and case 4 defined by the AIAA ADODG. We conclude that the GEK-based method is much more efficient than the traditional kriging-based method, and it has great potential for breaking or at least ameliorating the "curse of dimensionality" for higher-dimensional engineering design problems.

In the future, we will continue to make effort to improve the optimization efficiency and quality of GEK-based SBO, and perform optimizations on more complex cases with a larger number of design variables.

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