

SURROOPT: A GENERIC SURROGATE-BASED OPTIMIZATION CODE FOR AERODYNAMIC AND MULTIDISCIPLINARY DESIGN

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Abstract

Surrogate-based optimization (SBO) represents a type of optimization algorithm which makes use of surrogate models to approximate to the expensive objective and constraint functions, driving the adding and evaluation of new sample points towards the optimum. SBO has been shown to be very effective for engineering design problems where expensive numerical analysis such as computational fluid dynamics (CFD) is often employed. Despite the increasing popularity of SBO, it is seldom used as a generic optimization algorithm, due to its insufficient convergence properties, the difficulties associated with the so-called “curse of dimensionality”, as well as the incomplete functionalities of being a generic optimization algorithm. During the past decade, a number of researchers have continuously made effort to the development of SBO, towards an efficient global optimization algorithm which can solve arbitrary optimization problems with smooth, continuous design space. This paper reviews the recent progress in development of SBO in our research group, highlighting the development of a generic optimization code, “SurroOpt”, and its recent applications to aerodynamic and multidisciplinary design optimizations.

1 Introduction

During the past two decades, surrogate modeling played an important role in different areas of aerospace engineering, such as aerodynamic shape optimization, aerodynamic data production, structural design, and multidisciplinary design optimization (MDO) of aircraft or spacecraft. Surrogate-based optimization (SBO) represents a type of algorithm which makes use of surrogate models to approximate to expensive objective and constraint functions, throughout the design space or within the specific region, driving the adding and evaluation of new sample point(s) towards global or local optimum(s)(see [1][2][3]). SBO has been shown to be very effective for engineering design problems, in which expensive numerical analysis such as computational fluid dynamics (CFD) is often employed. Despite the increasing popularity of SBO, it is seldom used or viewed

as a generic optimization algorithm, due to its insufficient convergence properties, the difficulties associated with the so-called “curse of dimensionality”, as well as the incomplete functionalities of being a generic optimization algorithm. During the past decade, a number of researchers have made continuous effort to the development of SBO, towards an efficient global optimization algorithm which can be used to solve arbitrary optimization problems with continuous and smooth design space ^{[4][5][6]}. This paper reviews the recent progress in development of SBO in our research group, highlighting the development of a generic optimization code called “SurroOpt” and its recent applications to aerodynamic and multidisciplinary design optimizations.

SurroOpt is a research code developed for academic research and engineering designs driven by expensive numerical simulations. The distinguished feature is that building surrogate models and solving sub-optimization problems corresponding to the infill-sampling criteria are taken as a new 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 surrogate 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 surrogate models have less effect on the final optimum. We developed a series of algorithms and techniques to guarantee the convergence of SBO to local or global optimum and to improve the optimization efficiency for higher-dimensional problems, such as trust-region method, hybrid sub-optimization methods, etc. Constraint handling methods dedicated for SBO are developed, which makes it being well suited to engineering design problems with multiple constraints.

The remainder of the paper is organized as follows: section 2 reviews the theory and algorithms of SurroOpt; section 3 presents examples to show the performance of SurroOpt as well as its capability for aerodynamic and multidisciplinary design optimizations. The last section gives conclusions and outlook.

2 Surrogate-Based Optimization and Main Features of SurroOpt code

For an m -dimensional problem, suppose we are concerned with solving the following constrained optimization

$$\begin{aligned} &\text{Minimize } y(\mathbf{x}) \\ &\text{w.r.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u, \\ &\text{s.t. } g_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, N_C \end{aligned} \quad (1)$$

where $y(\mathbf{x})$ and $g_i(\mathbf{x})$ are the objective and constraint functions, respectively; N_C is the number of constraints; \mathbf{x}_u and \mathbf{x}_l are the lower and upper bounds of the design variables \mathbf{x} .

The framework of a typical SBO for solving the above optimization problem is sketched in Figure 1. Generally, a SBO process is consist of the following steps:

- 1) First, initial sample points are chosen by DoE method and the functional responses are evaluated by expensive numerical analysis code such as CFD solver.
- 2) Second, initial surrogate models for the objective and constraint functions are built, based on the sampled dataset.
- 3) Then, a full loop of sub-optimization defined by the infill-sampling criteria is executed based on the surrogate models, which in turn generates new sample points to be evaluated by expensive analysis code.
- 4) Fourth, the newly selected sample points as well as the functional responses are augmented to the sampling database and the surrogate models are updated.
- 5) Steps 3 and 4 are repeated until the termination condition is satisfied.

From the above procedure, one can see that the main ingredients of such a SBO process are: DoE method, surrogate modeling, infill-sampling criteria and sub-optimization, and termination conditions.

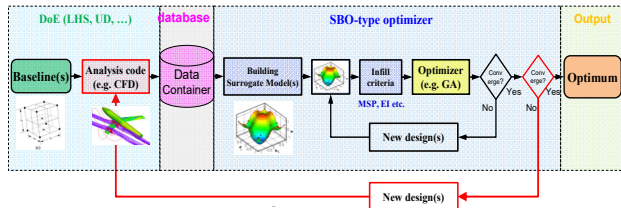


Figure 1. Framework of a typical SBO-type optimization

“SurroOpt” is a state-of-the-art, surrogate-based optimization code, which can be used to efficiently solve arbitrary single and multi-objective (Pareto front), unconstrained and constrained optimization problems. SurroOpt has built-in modern DoE methods suited for deterministic computer experiments, such as Latin hypercube sampling (LHS)^[7], uniform design (UD)^[8], and Monte Carlo design (MCD). A variety of surrogate models were developed such as quadratic response surface model (PRSM), kriging, gradient-enhanced kriging (GEK)^[9], hierarchical kriging (HK)^[10], cokriging^[11], radial-basis functions (RBFs), artificial

neutral network (ANN), support-vector regression (SVR) etc. A number of infill-sampling criteria and the dedicated constraint handling methods were implemented, such as minimizing surrogate prediction (MSP), expected improvement (EI), probability of improvement (PI), mean squared error (MSE), lower confidence bounding (LCB) and target searching (TS). Some well-accept and highly matured optimization algorithms, such as Hooke&Jeeves pattern search, BFGS quasi-Newton’s method, sequential quadratic programming (SQP), single/multi objective GAs, are employed to solve the sub-optimizations, in which the cost function(s) and constraint function(s) are evaluated by the cheap-to-evaluate surrogate models. In turn, new sample point(s) are generated and evaluated by the expensive analysis code. SurroOpt is mainly developed in Windows system and a branch has been created for Linux system. SurroOpt has been paralleled by MPI, which allows the user to run the code with multiple cores (or processors) to speed up the optimization. SurroOpt has a flexible user-defined interface, with which the user can set up their own optimization problems of interest. The main features of SurroOpt (version 2016) are listed in Table 1.

Table 1. List of main features of SurroOpt (version 2016), a generic surrogate-based optimization code

Sampling & opt.	DoE methods	Latin hypercube sampling(LHS) Uniform design(UD), Motel Carlo design (MCD)
	Infill-sampling method	MSP, EI (and local EI), PI, MSE, LCB, TS Combined infill sampling parallel infill sampling, e.g. q-EI, kriging believer (KB)
	Sub-optimizer	Hooke & Jeeves, single/multi objective GAs, BFGS, SQP
	Constraint handling	Probability method, e.g. constrained EI, PI, MSE,... Traditional methods, e.g. penalty function or SQP
	Multi-objective	Transform into single objective by linear weighting Pareto front
Surrogate modeling	Surrogate models	Polynomial response surface model (PRSM) Kriging (simple, ordinary, universal) Gradient-enhanced kriging (GEK) Cokriging Hierarchical kriging (HK) Radial-basis functions(RBFs) Support-vector regression (SVR), artificial neural network (ANN), polynomial chaos expansion (PCE) Variable-fidelity model (VFM) with additive, multiplicative and hybrid bridge functions
		Gaussian (GS) Gaussian exponential (GSE) Cubic spline (CUSP) Thin-plate spline (TPS) Power function (PS) Multi-quadratic (MQ) Inverse multi-quadratic (IMQ)
	Correlation or kernel functions	
Data & program	Data format	Tecplot, ASCII
	Program language	Fortran, C/C++, MPI, Python, Matlab
	Version control	SVN repository
	Operating system	Windows, Linux
	User-defined interface	" interface.f " , file I/O or library for importing the objective, constraint function values and gradients

2.1 Design of Experiments

To build a surrogate model, DoE method is usually used to determine a number of locations in the design space (called sampling sites) to be evaluated by numerical analysis code. DoE is a procedure with the general goal of maximizing the amount of information gained from a limited number of sample points^[7]. Currently, there are different DoE methods which can be classified into two categories^[7]: “classic” and “modern” DoE methods. The classic DoE methods, such as full-factorial design (FFD),

central composite design (CCD), Box-Behnken and D-optimal design (DOD), were developed for laboratory experiments. In contrast, the modern DoE methods such as Latin hypercube sampling (LHS), orthogonal array design (OAD) and uniform design (UD) were developed for design and analysis of deterministic computer experiments.

The DoE methods implemented in SurroOpt are the LHS, UD and MCD methods. More DoE method will be integrated in the future. Figure 2 shows an example of choosing 25 sample points by LHS and UD for a two-dimensional problem.

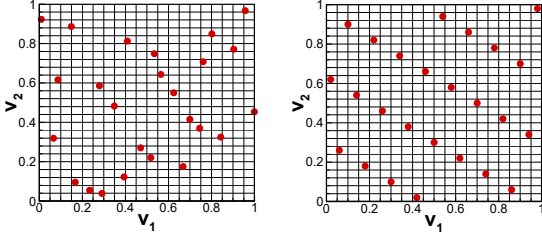


Figure 2. Schematics of 25 sample points chosen by Latin hypercube sampling (left) and uniform design (right) for a 2-D problem

2.2 Surrogate Models

For an m -dimensional problem, suppose we are concerned with the prediction of the output of a high-fidelity and expensive computer code, which corresponds to an unknown function $y: \mathbb{R}^m \rightarrow \mathbb{R}$. By running expensive numerical analysis, y is observed at n sites chosen by DoE

$$\mathbf{S} = [\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}]^T \in \mathbb{R}^{n \times m}, \mathbf{x} = \{x_1, \dots, x_m\} \in \mathbb{R}^m \quad (2)$$

with the corresponding responses

$$\mathbf{y}_s = [y^{(1)}, \dots, y^{(n)}]^T = [y(\mathbf{x}^{(1)}), \dots, y(\mathbf{x}^{(n)})]^T \in \mathbb{R}^n. \quad (3)$$

Surrogate modeling is such a procedure to build an approximation model $\hat{y}(\mathbf{x})$ based on the sampled dataset $(\mathbf{S}, \mathbf{y}_s)$

A variety of surrogate models are available in SurroOpt (see Table 1). They can be classified into two categories: parameterized and non-parameterized models. Parameterized models include polynomial response surface model (PRSM), polynomial chaos expansion (PCE). Non-parameterized models include kriging and its variants (e.g. gradient-enhanced kriging, hierarchical kriging and cokriging), radial-basis functions (RBFs), artificial neural network (ANN), support-vector regression (SVR). The reader is referred to [1]-[5] for the formulation and algorithms of the surrogate models.

2.3 Infilling-Sampling Criteria and Constraint Handling

Once the surrogate models are built, they can be used to guide the generation of new sample points by solving sub-optimization problems defined by infill-sampling criteria. The terminology of “infill-sampling criteria” [2][4][12] denotes “clever” ways of selecting new samples which are supposed to better than any of the existing sample points, and the terminology “sub-optimization” denotes the loop of solving the mathematical model defined by the infill-

sampling criteria. Since the objective and constraint functions are evaluated by cheap surrogate models, the computational cost is usually neglectable, compared to the expensive numerical analysis.

A number of infilling-sampling criteria is available in SurroOpt (see Table 2), such as minimizing the surrogate prediction (MSP) [4][14], maximizing the expected improvement (EI) [4][15][16], maximizing the probability of improvement (PI) [13][17][18], maximizing the mean squared error (MSE) [12][17], minimizing the lower confidence bound (LCB) [19], target searching (TS), etc.

Table 2. List of infill-sampling criteria implemented in SurroOpt (version 2016)

Infill-sampling criteria	Explanation	Mathematical model	Exploitation	Exploration
MSP	Minimizing surrogate prediction	$\text{Min. } \hat{y}(\mathbf{x})$ $\text{s.t. } \hat{g}_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, N_c$ $\mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$	✓	
EI	Maximizing expected improvement	$\text{Max. } E(I(\mathbf{x})) = \int_{-\infty}^{\infty} P[G_i \leq 0] dG_i$ $\text{s.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$	✓	✓
PI	Maximizing probability of improvement	$\text{Max. } P(I(\mathbf{x})) = \int_{-\infty}^{\infty} P[G_i \leq 0] dG_i$ $\text{s.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$	✓	
MSE	Maximizing mean squared error	$\text{Max. } MSE(\hat{y}(\mathbf{x})) = \int_{-\infty}^{\infty} P[G_i \leq 0] dG_i$ $\text{s.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$		✓
LCB	Minimizing lower-confidence bound	$\text{Min. } \hat{y}(\mathbf{x}) - \Delta \hat{y}(\mathbf{x})$ $\text{s.t. } \hat{g}_i(\mathbf{x}) \geq 0, \quad i = 1, \dots, N_c$ $\mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$	✓	✓
TS	Target searching	$\text{Max. } E(I_{\text{target}}(\mathbf{x})) = \int_{-\infty}^{\infty} P[G_i \leq 0] dG_i$ $\text{s.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u$	✓	✓

To explain how these criteria work, we use an example of a one-dimensional test function. A kriging surrogate model is built for the following function taken from [2], based four sample points $\mathbf{S} = [0, 0.4, 0.6, 1.0]^T$

$$y = (6x - 2)^2 \sin(12x - 4), x \in [0, 1]. \quad (4)$$

2.3.1 Minimizing Surrogate Prediction (MSP)

This is the most straightforward method. When surrogate models are built, they can be used to replace the expensive numerical analysis within the loop of a conventional gradient-based or gradient-free optimization process. The sub-optimization problem is defined as

$$\begin{aligned} &\text{Minimize } \hat{y}(\mathbf{x}) \\ &\text{w.r.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u, \\ &\text{s.t. } \hat{g}_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, N_c \end{aligned} \quad (5)$$

where $\hat{y}(\mathbf{x})$ and $\hat{g}_i(\mathbf{x})$ are the surrogate models for the objective and constraint functions, respectively. A hybrid method of combining GA, Hooke&Jeeves pattern search and gradient-based method is used to solve the above sub-optimization, and then an optimum \mathbf{x}^* is obtained. To enhance the local convergence of MSP, a trust-region method can be used. The new sample site \mathbf{x}^* is evaluated by expensive numerical analysis and the functional responses together with \mathbf{x}^* are augmented to the sampling database to update the surrogate models. The procedure of building surrogate models, sub-optimization, and evaluation of new sample point is repeated until termination condition is satisfied.

The minimum upon the surrogate model for the 1D test function is shown in Figure 3, where red circles represent the sample points, blue dash double-dotted line

stands for the surrogate model built from the sample points, and the red filled-circle is the minimum upon the surrogate model, which is taken as the new sample point.

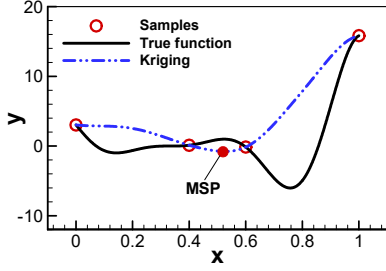


Figure 3. Schematics of MSP infilling-sampling criterion for a 1D problem

2.3.2 Expected Improvement (EI)

This method was proposed by Jones et al.^[16] in 1998. The surrogate-based optimization using EI criterion is also known as the efficient global optimization (EGO) method. Assume that the best observed object function as far is y_{\min} and the prediction of a kriging model coincides a Gaussian normal distribution with mean of $\hat{y}(\mathbf{x})$ and standard deviation of $s(\mathbf{x})$, i.e. $\hat{Y}(\mathbf{x}) \in N[\hat{y}(\mathbf{x}), s^2]$. The probability density function is

$$P(\hat{Y}(\mathbf{x})) = \frac{1}{\sqrt{2\pi} s(\mathbf{x})} \exp\left(-\frac{1}{2} \left(\frac{Y(\mathbf{x}) - \hat{y}(\mathbf{x})}{s(\mathbf{x})}\right)^2\right). \quad (6)$$

For a minimization problem, the statistical improvement is defined as

$$I(\mathbf{x}) = \max(y_{\min} - \hat{Y}(\mathbf{x}), 0). \quad (7)$$

And the expectation of the improvement function is

$$E[I(\mathbf{x})] = \begin{cases} (y_{\min} - \hat{y})\Phi\left(\frac{y_{\min} - \hat{y}}{s}\right) + s\phi\left(\frac{y_{\min} - \hat{y}}{s}\right) & \text{if } s > 0 \\ 0 & \text{if } s = 0 \end{cases}, \quad (8)$$

where $\Phi(\cdot)$ and $\phi(\cdot)$ are cumulative distribution and probability density functions of a standard normal distribution, respectively.

The computation of EI for the 1D test function is illustrated in Figure 4, where $P(\hat{Y})$ is the probability density function predicted by the kriging surrogate model, the blue shaded area denotes the probability of improvement $P[I(\mathbf{x})]$ and the integral of $I(\mathbf{x}) \cdot P(\hat{Y})$ with respect to $I(\mathbf{x})$ over the blue shaded area gives $E[I(\mathbf{x})]$. The red solid line represents the distribution of EI function in the design space.

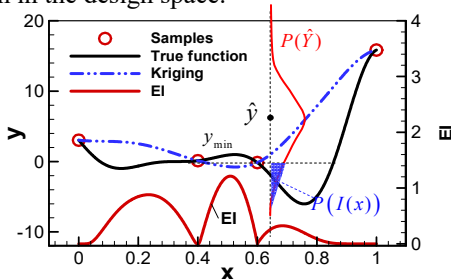


Figure 4. Schematics of EI function for a 1D problem

For a constrained optimization problem, one can also build surrogate models for the constrained functions $\hat{g}_i(\mathbf{x})$, and assume that the corresponding random variable $G_i(\mathbf{x})$ is normally distributed, with mean of $\hat{g}_i(\mathbf{x})$ and standard derivation of $s_{g,i}(\mathbf{x})$. The probability of satisfying the constraint at any site can be calculated as

$$P[G_i(\mathbf{x}) \leq 0] = \Phi\left(-\frac{\hat{g}_i(\mathbf{x})}{s_{g,i}(\mathbf{x})}\right). \quad (9)$$

Then the sub-optimization problem can be defined as

$$\begin{aligned} & \text{Maximize } E(I(\mathbf{x})) \cdot \prod_{i=1}^{N_c} P[G_i \leq 0], \\ & \text{w.r.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u \end{aligned} \quad (10)$$

which is a global optimization problem with multiple local extra. In SurroOpt, we use a hybrid of GA, multi-starting-point Hooke&Jeeves and gradient-based methods to solve above sub-optimization and get the optimum site \mathbf{x}^* . Practice suggests that this hybrid strategy enables us to find more accurate solution, which in turn accelerates the main optimization process by reducing the calls of expensive numerical analysis. To enhance the local convergence, we also proposed a method called “local EI” to search for the maximum EI in the neighbored region of the current best. The new sample site \mathbf{x}^* is evaluated by expensive numerical analysis again and the surrogate models are rebuilt. The procedure is repeated until termination condition is satisfied.

2.3.3 Probability of Improvement (PI)

Instead of maximizing the expected improvement, one can also maximize the probability of improvement (PI). According to Eq.(6), the PI function can be calculated by

$$P[I(\mathbf{x})] = \Phi\left(\frac{y_{\min} - \hat{y}(\mathbf{x})}{s(\mathbf{x})}\right). \quad (11)$$

For the 1D test case, the PI function (the red solid line) is sketched in Figure 5.

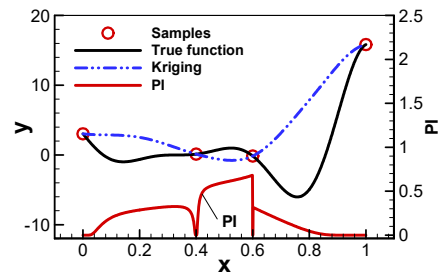


Figure 5. Schematics of PI function for a 1D problem

For constrained optimization, one can use a similar way to the constrained EI method and solve the following sub-optimization

$$\begin{aligned} & \text{Maximize } P(I(\mathbf{x})) \cdot \prod_{i=1}^{N_c} P[G_i \leq 0] \\ & \text{w.r.t. } \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u \end{aligned} \quad (12)$$

to get the new sample sits \mathbf{x}^* .

2.3.4 Mean Squared Error (MSE)

To fully explore the design space, there is a criterion of maximizing MSE to improve the global accuracy of surrogate models. The root MSE of the 1D test function (red solid line) is shown in Figure 6. For constrained optimization, the following sub-optimization is solved

$$\begin{aligned} & \text{Maximize} \quad MSE(\hat{y}(\mathbf{x})) \cdot \prod_{i=1}^{N_c} P[G_i \leq 0] \\ & \text{w.r.t.} \quad \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u \end{aligned} \quad (13)$$

to get the new sample sits \mathbf{x}^* .

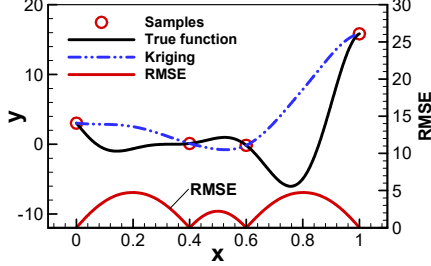


Figure 6. Schematics of RMSE function for a 1D problem`

2.3.5 Lower Confidence Bound (LCB)

In addition to EI, PI, and MSE, another kind of method making use of the uncertainty of kriging prediction is called LCB^[19], which was proposed in 1998. Recall that the prediction of a kriging model can be viewed as a normal distribution with mean of $\hat{y}(\mathbf{x})$ and standard deviation of $s(\mathbf{x})$, one can minimize the lower confidence bound of the kriging prediction to get the new sample site \mathbf{x}^* . LCB function (also see [2][12]) is defined as :

$$LCB(\mathbf{x}) = \hat{y}(\mathbf{x}) - A \cdot s(\mathbf{x}), \quad (14)$$

where A is a user-defined parameter to balance the exploitation and exploration. When $A \rightarrow 0$, $LCB \rightarrow \hat{y}(\mathbf{x})$ the LCB reverts to a MSP, in which the surrogate model prediction is directly minimized; when $A \rightarrow \infty$, $LCB \rightarrow s(\mathbf{x})$, the LCB is identical to a MSE criterion, which is a pure exploration. Out best practice is to set A in the range from 1 to 4. The LCB (red solid line and $A = 1$) for the 1D test function is sketched in Figure 7.

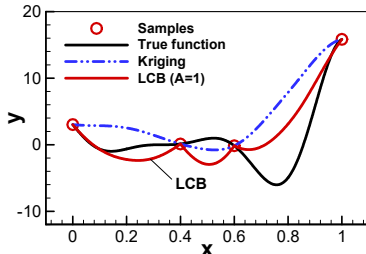


Figure 7. Schematics of LCB function for a 1D problem

For constrained optimization, one can solve the following sub-optimization

$$\begin{aligned} & \text{Minimize} \quad \hat{y}(\mathbf{x}) - A\hat{s}(\mathbf{x}) \\ & \text{w.r.t.} \quad \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u, \\ & \text{s.t.} \quad \hat{g}_i(\mathbf{x}) \leq 0, i = 1, \dots, N_c \end{aligned} \quad (15)$$

to get the new sample sits \mathbf{x}^* .

2.3.6 Target Searching (TS)

If one roughly know the value of the best objective function, y_{target} , the goal of the sub-optimization can be set to achieve or exceed this target value. For example, we can calculate the expected improvement over this target, rather than over the best among the observed sample points. The idea is similar to the goal seeking (GS) using conditional likelihood method (see [2]). The statistic improvement is redefined as

$$I_{\text{target}}(\mathbf{x}) = \max(y_{\text{target}} - \hat{y}(\mathbf{x}), 0). \quad (16)$$

Then we obtain the expected improvement for target searching

$$E[I_{\text{target}}(\mathbf{x})] = \begin{cases} (y_{\text{target}} - \hat{y})\Phi\left(\frac{y_{\text{target}} - \hat{y}}{s}\right) + s\phi\left(\frac{y_{\text{target}} - \hat{y}}{s}\right) & \text{if } s > 0. \\ 0 & \text{if } s = 0 \end{cases} \quad (17)$$

2.3.6 Combined and Parallel Infill-Sampling Criteria

The infill-sampling criteria can be combined to overcome the drawback of a single criterion. For example, we can use MSP and EI to select two sample points at each updating cycle. Note that different combination of infill-sampling criteria can be used in SurroOpt. To further improve the optimization efficiency, a single criterion can be paralleled by selecting multiple points, which are evaluated by numerical analysis code in parallel. Some popular methods such as q-EI and “kriging believer” method were implemented in SurroOpt.

2.4 Multi-Objective Optimization

For multi-objective optimization, two kinds of method were implemented in SurroOpt. The first method is a linear weighting method to transform the multi-objective optimization to a single-objective optimization. The weighted objective function is

$$y = w_1 y_{\text{obj}1} + w_2 y_{\text{obj}2} + \dots + w_n y_{\text{obj}n}. \quad (18)$$

Then we build surrogate model for it and execute SBO in a same way as the single-objective optimization. The second kind of method is Pareto front optimization. First we build surrogate models for all the objective and constraint functions; then we use multi-objective genetic algorithm NSGAII to solve the sub-optimization below

$$\begin{aligned} & \text{Minimize} \quad \hat{y}_{\text{obj}1}(\mathbf{x}), \hat{y}_{\text{obj}2}(\mathbf{x}), \dots, \hat{y}_{\text{obj}n}(\mathbf{x}) \\ & \text{w.r.t.} \quad \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u \\ & \text{s.t.} \quad \hat{g}_i(\mathbf{x}) \leq 0, \quad i = 1, \dots, N_c \end{aligned} \quad (19)$$

to get a group of new sample points, which are then evaluated by expensive analysis code and used to update the surrogate model, driving the process towards a final Pareto front solution. Other methods using EI, LCB functions are also available, but not fully tested.

2.5 Termination Conditions and Restart

Four termination conditions were defined in SurroOpt. The first one is about the distance between samples and difference of their objective responses

$$\begin{aligned} \|\mathbf{x}_{new} - \mathbf{x}_{best}\| / \|\mathbf{x}_{best}\| &\leq \varepsilon_1 \\ |y_{new} - y_{best}| / |y_{best}| &\leq \varepsilon_2 \end{aligned} \quad (20)$$

The second one is about the approximation accuracy of surrogate model

$$|\hat{y}_{best} - y_{best}| / |y_{best}| \leq \varepsilon_3. \quad (21)$$

The third one is about the maximum number of expensive function evaluations

$$N \leq N_{\max}. \quad (22)$$

The fourth is a specific one for EI infill-sampling criterion

$$\max(EI) \leq \varepsilon_4. \quad (23)$$

In general, if one of above conditions is reached, the optimization is terminated.

SurroOpt has a nice feature of restart. The optimization can be terminated and necessary information for restart will be stored. It is very convenient for the user to continue the optimization from the last termination point, just setting $\text{restart} = 1$.

2.6 Flowchart of SurroOpt

The flowchart of SurroOpt is sketched in Figure 8. Note that the code has been paralleled by MPI and a user-define interface can be used to set up their own problems of interest.

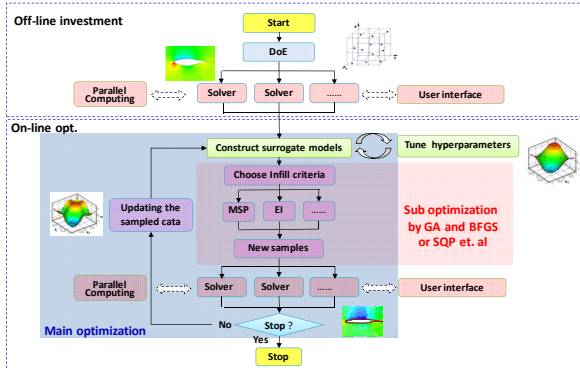


Figure 8. Flowchart of SurroOpt, a generic optimization code

3 Examples

3.1 Benchmark Analytical Test Cases

Four analytical test cases are used to validate and demonstrate the SurroOpt code.

3.1.1 Rastrigin Test Case

Here we test SurroOpt for a two-dimensional unconstrained global optimization problem (see Figure 9 for the landscape of 2D Rastrigin function). The mathematical model is

$$\begin{aligned} \text{Minimize } f(\mathbf{x}) &= 10 \times 2 + \sum_{i=1}^2 [x_i^2 - 10 \times \cos(2\pi x_i)] \\ \text{w.r.t. } x_i &\in [-5.12, 5.12], \quad i = 1, \dots, 2 \end{aligned} \quad (24)$$

The theoretical optimal solution is at $(x_1^*, x_2^*) = (0, 0)$ and with $f(x_1^*, x_2^*) = 0$. Four sample points are chosen by DoE to build the initial surrogate model. The convergence

histories of the objective function of using different infill-sampling criteria as well as combined criteria is shown in Figure 10. By using EI, LCB and different combined criteria, SurroOpt successfully finds the global optimum, but fails when using single criteria of MSP, MSE or PI. It is also observed that both “MSP+EI” and “MSP+LCB” have great performance in this test case.

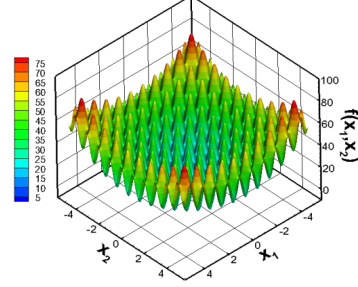


Figure 9. Schematics of 2D Rastrigin function

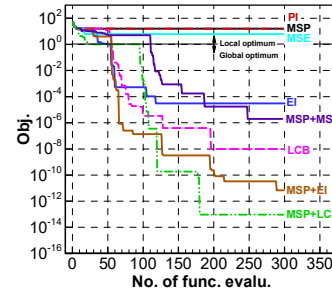


Figure 10. Convergence histories of using different infill-sampling criteria for 2D Rastrigin test case

3.1.2 G9 test case

This is benchmark test case for strongly constrained global optimization [20]. The mathematical model is

$$\begin{aligned} \text{Minimize } f(\mathbf{x}) &= (x_1 - 10)^2 + 5(x_2 - 12)^2 + x_3^4 + 3(x_4 - 11)^2 \\ &\quad + 10x_5^6 + 7x_6^2 + x_7^4 - 4x_6x_7 - 10x_6 - 8x_7 \\ \text{w.r.t. } x_i &\in [-10, 10], \quad i=1, \dots, 7 \\ \text{s.t. } g_1 &= -127 + 2x_1^2 + 3x_2^4 + x_3 + 4x_4^2 + 5x_5 \leq 0 \\ g_2 &= -282 + 7x_1 + 3x_2 + 10x_3^2 + x_4 - x_5 \leq 0 \\ g_3 &= -196 + 23x_1 + x_2^2 + 6x_6^2 - 8x_7 \leq 0 \\ g_4 &= 4x_1^2 + x_2^2 - 3x_1x_2 + 2x_3^2 + 5x_6 - 11x_7 \leq 0 \end{aligned} \quad (25)$$

There are 7 design variables and 4 constraints, in which the first and last ones are active constraints. This is very difficult optimization since the feasible region is only 0.5% of the design space and the value of the objective function ranges from hundreds to ten millions. Although the real optimum is unknown, the optimization community has observed a best solution of

$$\begin{aligned} \mathbf{x}^* &= (2.330499, 1.951372, -0.4775414, 4.365726, \\ &\quad -0.6244870, 1.038161, 1.594227) \\ f(\mathbf{x}^*) &= 680.6300573 \end{aligned} \quad (26)$$

which is taken as a reference for comparison. Fourteen initial sample points are chosen to build initial surrogate models. The results of using different in-filling sampling criteria are shown in Table 4. It is observed that the combined criterion “MSP+EI” gets the best objective functional of 680.64287, which is very close to the reference value of 680.63006. The results and efficiency of using SurroOpt is compared with GA, which shows that SurroOpt is much more efficient, with respect to

number of functional evaluations. The best results of using SurroOpt are compared with the reference in Table 4. It can be observed that, for the reference, the last constraint ($g_4=0.00014$) is actually violated a little bit, but all the constraints are strictly satisfied when using SurroOpt, which explains why the optimal objective function obtained by SurroOpt is slightly larger than the reference value.

Table 3. Comparison of different methods for G9 benchmark test case, a strongly constrained global optimization

Opt. algorithms	Best objective	Number of function evaluations
Best observed so far	680.63006	n/a
Kriging MSP	688.41155	175
Kriging EI	680.66619	1331
Kriging local EI	680.82861	1011
Kriging LCB	689.65021	401
Kriging MSP+EI	680.64287	1009
Kriging MSP+LCB	684.72006	402
Kriging MSP+MSE	687.90582	987
GA	681.00720	21000

Table 4. Optimal results of G9 test case using combined MSP and EI infill-sampling criteria

Opt algorithms	Optimum design variables	Best obj.
SurroOpt	$x^* = (2.3331998, 1.942837, -0.479546, 4.387811, -0.632617, 1.039775, 1.600996)$	680.64287
Best observed so far	$x^* = (2.330499, 1.951372, -0.4775414, 4.365726, -0.6244870, 1.038161, 1.594227)$	680.63006
Constraint at optimal point		
SurroOpt	$g_1 = -0.000259$ $g_2 = -252.519016$ $g_3 = -144.882960$ $g_4 = -0.00133$	
Best observed so far	$g_1 = -0.000043$ $g_2 = -252.561721$ $g_3 = -144.877817$ $g_4 = 0.00014$	

3.1.3 TNK Multi-Objective Test Case

TNK is a 2D constrained multi-objective optimization, whose mathematical model is

$$\begin{aligned}
 &\text{Minimize } f_1(x) = x_1, f_2(x) = x_2 \\
 &\text{w.r.t. } x_i \in [0, \pi], i = 1, 2 \\
 &\text{s.t. } g_1(x) = -x_1^2 - x_2^2 + 1 + 0.1 \cos(16 \arctan(x_1/x_2)) \leq 0 \\
 &\quad g_2(x) = (x_1 - 0.5)^2 + (x_2 - 0.5)^2 - 0.5 \leq 0
 \end{aligned} \quad (27)$$

In Table 5, the optimal Pareto front by SurroOpt is compared to the true optimum and those by directly using NSGAII, which validates the functionality of Pareto front optimization of SurroOpt. Further comparison with NSGAII is conducted and illustrated in Table 5, with respect to number of Pareto front points, convergence and diversity of the front, and number of function evaluations. It can be seen that the number of function evaluation of using SurroOpt is much less than that of using NSGA II, when reaching a comparable level of solution quality.

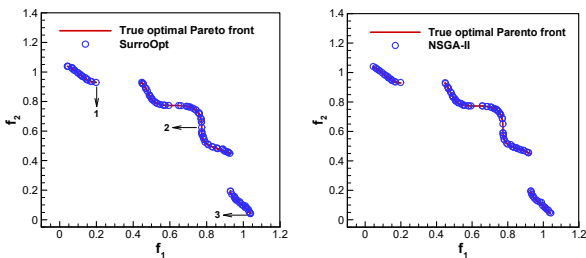


Figure 11. Comparison of Pareto fronts obtained by using SurroOpt and NSGAII for a TNK test case

Table 5. Comparison of Pareto front solutions obtained by SurroOpt and NSGA II for TNK test case

Opt. algorithms	No. of Pareto front solutions	Convergence	Diversity	No. of function evaluations
SurroOpt (repeat 30 times)	112	1.6978E-3	0.625964	278
NSGA-II (repeat 30 times)	100	1.7136E-3	0.657046	20000

3.1.4 MDO test case

Note that, as a generic optimizer, SurroOpt (version 2016) is able to deal with both inequality and equality constraints. Hence, we can use SurroOpt as the optimizer in different MDO architectures^[22], such as multidisciplinary design feasible (MDF), individual design feasible (IDF) and simultaneous analysis and design (SAND), collaborative optimization (CO), concurrent subspace optimization (CSSO), etc.

An analytical test case by Sellar^[21] is employed to demonstrate SurroOpt in different MDO architectures. The optimization problem is defined as

$$\begin{aligned}
 &\text{Minimize } f(x_1, x_2, x_3) = x_2^2 + x_3 + y_1 + e^{-y_2} \\
 &\text{w.r.t. } -10 \leq x_1 \leq 10, 0 \leq x_2, x_3 \leq 10 \\
 &\text{s.t. } g_1 = 8 - y_1 \leq 0 \\
 &\quad g_2 = y_2 - 10 \leq 0
 \end{aligned} \quad (28)$$

There are two disciplines. One is given by,

$$y_1 = x_1^2 + x_2 + x_3 - 0.2y_2, \quad (29)$$

and the other is given by

$$y_2 = \sqrt{y_1} + x_1 + x_3. \quad (30)$$

The global optimum is located at (3.0284, 0, 0) and has a best objective of 8.00286. For clarity, the coupling of the discipline is sketched in Figure 12.

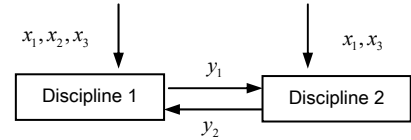


Figure 12. Schematics of two coupled disciplines for a MDO test case

The results are presented in Table 6 and compared with those obtained by a gradient-based method. It is shown that SurroOpt successfully solves this MDO problem with different architectures, and needs less number of function evaluations both in system and disciplinary levels.

Table 6. Comparison of SurroOpt and gradient-based method for an analytical MDO test case

Opt. methods	MDO architectures	Optimum objective and constraint functions			Number of function evaluations		
		Obj.	g_1	g_2	MDA	Disciplinary 1	Disciplinary 2
SBO via SurroOpt (2016)	MDF	8.002860238	-1.10e-8	-4.14315	22	95	95
	IDF	8.002860326	-9.27e-6	-4.14313	0	33	33
	SAND	8.002860225	-8.84e-10	-4.14314	0	35	35
Gradient-based method	MDF	8.002860227	-1.78e-15	-4.14315	32	284	284
	IDF	8.002860227	1.75e-8	-4.14316	0	61	61
	SAND	8.002860227	0	-4.14315	0	67	67

3.2 Aerodynamic Shape Optimization

3.2.1 Airfoil Design

This is a benchmark test case (case 2) defined by AIAA aerodynamic design optimization discussion

group (ADODG). The objective is to minimize the drag of an RAE 2822 airfoil, subject to lift, pitching moment and sectional area constraints. The design sate is $Ma = 0.734$ $Re = 6.5 \times 10^6$. The mathematical model is of the form

$$\begin{aligned} & \text{Minimize } C_d \\ & \text{s.t. } C_l = 0.824, \\ & |C_m| \leq 0.092, \\ & A \geq A_0 \end{aligned} \quad (31)$$

where C_l, C_d, C_m represent lift, drag, and moment coefficients, respectively; A, A_0 stand for the sectional areas of optimal and baseline airfoils, respectively. After grid convergence study, we used a grid of 512×256 , as sketched in Figure 13(left). The convergence history of the drag w.r.t. number of RANS (Reynolds-averaged Navier-Stokes) simulations is shown in Figure 13(right). The pressure distributions and geometric shapes of the baseline and optimal airfoils are shown in Figure 14. The aerodynamic performances before and after optimization are illustrated in Table 7, which shows that the drag is dramatically reduced and all the constraints are satisfied.

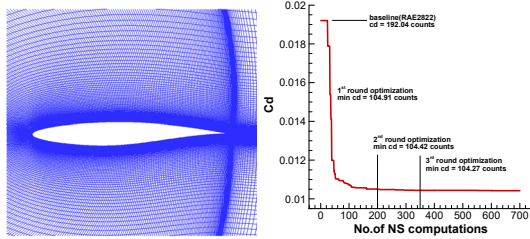


Figure 13. Computational grid (left) and convergence history (right) for drag minimization of benchmark RAE 2822 airfoil test case

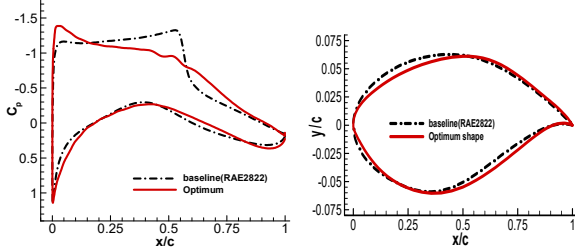


Figure 14. Comparison of pressure distributions (left) and geometries (right) for baseline and optimal airfoils

Table 7. Comparison of performances of baseline and optimum airfoils

Airfoils	C_l (counts)	C_d (counts)	C_m	A
Baseline	82.4	195.00	-0.0921	0.07794
Optimal	82.4	104.29	-0.0880	0.07794

3.2.2 Wing Design

As a three-dimensional aerodynamic shape optimization, the objective is to minimize the drag for the ONERA M6 wing, parameterized with 30 design variables (4 for platform shape and 26 for shapes of two control sections). The design point is at the free-stream condition of $Ma = 0.8395$, $Re = 11.72 \times 10^6$, $\alpha = 3.06^\circ$. The constraints are associated with the lift coefficient, maximum thickness-to-chord ratio of the root and tip sections, and area of the wing. The following formula gives the mathematical model of optimization

$$\begin{aligned} & \text{Minimize } C_d \\ & \text{s.t. } C_l \geq C_{l0} \\ & Thick_r \geq Thick_{r0} \\ & Thick_t \geq Thick_{t0} \\ & Area \geq Area_0 \end{aligned} \quad (32)$$

The computational grid and the geometric parametrization are sketched in Figure 15. The convergence history of drag w.r.t. number of RANS simulations is shown in Figure 16. One can see that although none of the initial sample point is feasible, SurroOpt is able to drive the searching of feasible new designs with reduced drag. It is also shown that the parallel infill-sampling method of choosing 4 samples simultaneously is more efficient than the EGO method [16], in which only one sample point is chosen at each update cycle. The pressure contours for baseline and optimized wings are compared in Figure 17, which shows that the shock waves are smoothed out. The sectional pressure distributions at two span-wise locations (37.6% and 72.7% semi-spans, see Figure 18) also confirm the suppression of shock waves.

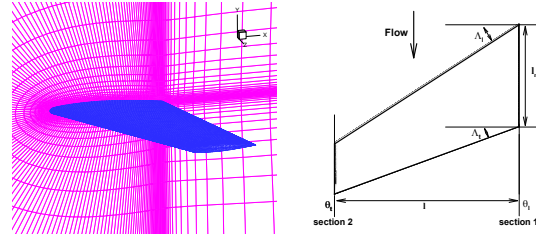


Figure 15. Computational grid (left) and geometric parameterization (right) for drag minimization of M6 wing (30 design variables)

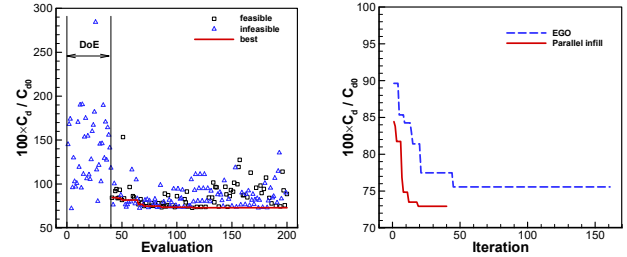


Figure 16. Convergence history of objective function for drag minimization of M6 wing (left) and comparison of single EI and parallel infill-sampling methods (right)

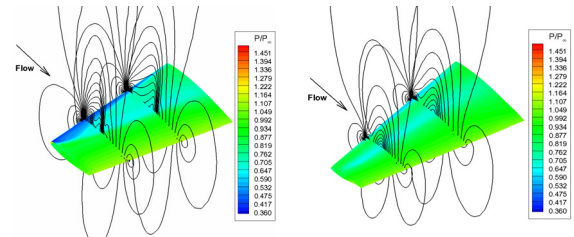


Figure 17. Comparison of pressure contours for baseline M6 and the optimized wings (surface and sectional at 37.6%, 72.7% semi-spans)

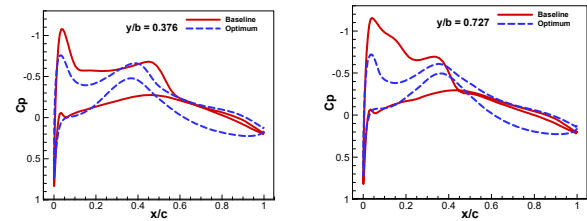


Figure 18. Comparison of pressure distributions for baseline M6 and optimized wings (left: 37.6% half span; right: 72.7% half span)

The aerodynamic and geometric performances of the baseline and optimized wings are listed in Table 8, which shows that drag coefficient is reduced by 27.07% after 200 RANS simulations. Please note again that all the constraints are strictly satisfied, which indicates that SurroOpt has a good capability of constraint handling.

Table 8. Comparison of aerodynamic force coefficients and geometric parameters of baseline M6 and optimized wings

	Baseline	Optimum
C_d	0.01751	0.01277 (-27.07%)
C_l	0.23803	0.23814 (+0.05%)
$Thick_x$	0.09786	0.09786 (+0.00%)
$Thick_y$	0.09786	0.10021 (+2.40%)
Area	0.75318	0.75529 (+0.28%)

In addition to the M6 wing, SurroOpt has been applied to aerodynamic shape optimization of transport aircraft wing, flying wing as well as helicopter rotors, blades of propeller and wind turbines, with number of design variables in the range from 30 to 52. The results are not given here due to the limited length of the paper.

3.2 Multidisciplinary Design Optimization

SurroOpt (version 2016) was tested for aerodynamic/structural integrated design of the wing of a wing-body configuration, representative of a high-subsonic transport aircraft (see Figure 19). The aircraft is cruised at an altitude of 10km and Mach number of 0.76; the wing area is $105m^2$. The aerodynamic shape and structural layout of the wing are parameterized with 23 design variables. The mathematical model is

$$\begin{aligned}
 &\text{Minimize } W_{wing} \\
 &\text{s.t. } L \geq 54 \text{ ton} \\
 &\quad L/D \geq 27, \\
 &\quad \sigma_{max} \leq [\sigma] \\
 &\quad \delta_{max} \leq 1 \text{ m}
 \end{aligned} \quad (33)$$

where W_{wing} is structural weight of single wing; L and L/D are the lift and lift-to-drag ratio of the wing-body configuration, respectively; σ_{max} and δ_{max} are maximum equivalent stress and wing deformation, respectively. The design variables are cruise angle of attack, taper ratio of the wing, linear twist angle and the thickness distribution of skin along the wing span (20 variables). The detailed description about the aerodynamic and structure analysis models can be found in [23]. MDF architecture is used to solve this MDO problem. Note that within the MDF architecture, a complete MDA (multidisciplinary design analysis) involves a full static aeroelasticity analysis, in which aerodynamic and structural analysis are coupled with a loose coupling strategy, until both the aerodynamic force and structural deformation converge.

200 hundred of initial sample points are generated by LHS and evaluated by MDA. The initial surrogate models for the objective and constraint functions are built and repetitively updated by selecting new sample points, through the sub-optimizations using the combination of MSP and EI criteria. The optimization converges after 50 iterations (see Figure 20), which means that the total number of MDAs is around 300. A detailed performance comparison of baseline and optimized configurations can

be found in Table 9. It is shown that, by using SurroOpt, the wing weight is significantly reduced, while the aerodynamic characteristics are maintained. A comparison of deformations and skin thinness distributions of baseline and optimized wings is sketched in Figure 21.

In the future, more design variables and constraints as well as higher-fidelity of MDA will be adopted to refine the optimization.

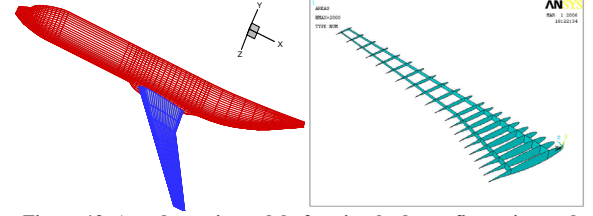


Figure 19. Aerodynamic model of a wing-body configuration and structural layout of wing for a high-subsonic transport aircraft

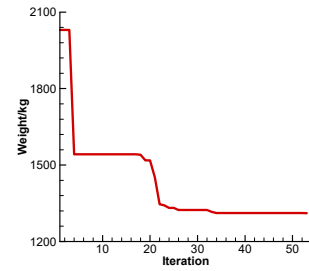


Figure 20. Convergence history of MDO of the wing of a wing-body configuration representative of a transport aircraft.

Table 9. Performance of the baseline and optimum configurations for a wing-body configuration

Features of wing	Baseline	Optimized
Taper ratio of wing	0.21	0.21
Linear twist angle of wing /deg.	-2.49	-4.00
Cruise angle of attack /deg.	0.82	1.03
Wing weight/kg	2030.3	1311.1
Lift /ton	61345.8	54003.4 (>54 ton)
Lift-to-drag ratio	27.56	27.01 (>27)
Max. equivalent stress/ 10^6 pa	2.7327	2.7282
Max. deformation of wing /m	0.947	0.998 (<1m)

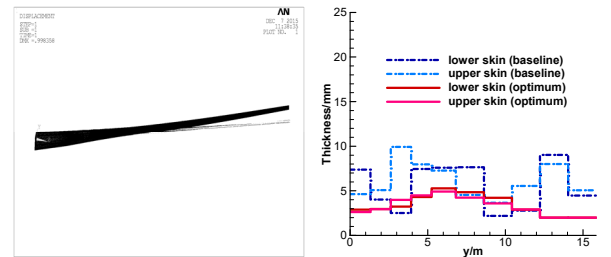


Figure 21. Comparison of deformations and skin thinness distributions of baseline and optimized wings for a transport aircraft

4 Conclusions and Outlook

This paper summarizes the development of a surrogate-based optimization code called SurroOpt and its recent applications to aerodynamic and multidisciplinary design optimization of aircraft. The main ingredients including DoE, surrogate models, infill-sampling criteria and sub-optimization, and termination conditions are introduced.

SurroOpt were intensively tested for benchmark optimization test cases and has been successfully applied to aerodynamic design of airfoils, wings, propellers, helicopter rotors and wind turbines, as well as multidisciplinary design optimization of transport wings. Some conclusions about SurroOpt can be drawn as:

- 1) SurroOpt is suited for engineering designs driven by expensive numerical analysis. It is capable of finding global (or at least more global) optimum, and is much more efficient than genetic algorithms.
- 2) For the test cases with number of design variables in the range from 2 to 52, SurroOpt usually gives good design within 300 expensive numerical simulations.
- 3) There are a number of infill-sampling criteria and hybrid sub-optimizations in SurroOpt. Combined or parallel infill-sampling are also available for improving the optimization efficiency. Practices suggest that using the combination of MSP and EI can generally give good and robust convergence.
- 4) SurroOpt has the functionality of Pareto front multi-objective optimization. A TNK test case shows that it is much efficient than NSGAI w.r.t. to number of expensive function evaluations.
- 5) SurroOpt has a good capability of constraint handling. For all the test cases, the constraints are strictly satisfied. A new functionality of handling equality constraint was developed and successfully applied in MDO architectures of IDF and SAND.

In the future, we will continue to improve the optimization efficiency and quality of SurroOpt, and adapt it to more computer architectures. More functionalities or innovative algorithms will be integrated and special attentions will be paid to gradient-enhanced and variable-fidelity surrogate models, towards efficient global optimization with larger number of design variables (>100) and many constraints. Robust design under uncertainties and MDO applications will be important concerns for future development.

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