Hybrid Single and Multiobjective Optimization for Engineering Design without Exact Specifications

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***Abstract*—A challenge in engineering design optimization is that sufficient information may not be available to define the exact specifications beforehand. While iterative trial optimization using different specifications is widely used in industry, multiobjective optimization is attracting much attention in the academic field. However, off-the-shelf methods in both categories are time-consuming due to the involved computationally expensive simulations. In this paper, the characteristics of the targeted problem are summarized; the gap between off-the-shelf methods and the practical need is then analyzed. A simple yet effective framework, called two-stage multi-fidelity surrogate model-assisted optimization (TMSO), is proposed to improve efficiency. TSMO is implemented by two state-of-the-art optimization algorithms and two real-world design cases demonstrate its effectiveness in practice. The research topics in multiobjective optimization and surrogate model-assisted optimization inspired by the TSMO framework is finally discussed.**

***Index Terms*—multi-fidelity optimization, engineering optimization, multiobjective, simulation-based optimization, surrogate model, MOEA/D, surrogate model-aware evolutionary search**

I. Introduction

Engineering design often follows the top-down design flow [1], including system-level design and building block-level design. The whole (sub)system is firstly divided into a number of building blocks, each of which has a behavioral model. Based on the behavioral models, design specifications are coarsely allocated to each of the building blocks. With the assigned specifications, the building block-level design can often be formulated as a simulation-based optimization problem. The example of an analog-to-digital converter design is as follows: the converter (i.e., system) is firstly decomposed into a certain number of amplifiers and comparators (i.e., building blocks), and a set of approximate design specifications is set to each of them. For the more than ten design specifications of an amplifier, most of them are not exact. For instance, the phase margin should be around 60°; 55° can still be used although not preferred; higher than 70° is not necessary. Using these design specifications, the transistor implementation will be carried out, which is a simulation-based optimization problem [2] and is the target of this paper.

This optimization is not trivial because of the following two reasons: (1) the involved simulation is often computationally expensive; (2) the specifications assigned to each building block are often inexact like the above example. It is clear that excessively strict specifications may cause the optimization to fail, whereas overly relaxed specifications may not obtain design solutions with sufficient quality. To address the above challenges, the closely related research in the computational intelligence field are surrogate model-assisted evolutionary algorithms (SAEAs) and multiobjective evolutionary algorithms (MOEAs).

To cope with the computationally expensive simulations, surrogate models are employed. Surrogate models are computationally cheap approximation models predicting the response from design parameters, which are often constructed by statistical learning techniques. By replacing computationally expensive simulations to computationally cheap surrogate model predictions, the optimization time can be substantially reduced. Surrogate model predictions have errors, which may mislead the optimization. The way to make surrogate models and optimization work harmoniously is the key of SAEA, which is called model management [3]. Using different model management methods, different SAEAs are produced.

To cope with the inexact design specifications, the way that is widely used in industry is trial-and-error. Different design specifications are tried assisted by design experience to find the appropriate ones and thus the optimal design. This often leads to a number of trial optimization runs, especially when there are many specifications. The other way that is well investigated in the computational intelligence field is multiobjective optimization [4]. A Pareto front (PF) is generated showing optimal trade-offs of different design specifications. Designers can then select a design that best fits their interests. Note that the computing overhead of MOEAs is much higher than single objective evolutionary algorithms (EAs). To improve efficiency, surrogate model-assisted MOEAs [5] and interactive MOEAs [6] are introduced. Although surrogate modeling and iterative selection of region of interest (ROI) in the multiobjective optimization save much computing overhead, the optimization time is still very long [4].

This paper aims at identifying the gap between off-the-shelf methods in MOEA research and practical need for engineering design problems, providing an efficient optimization framework for the targeted problem as well as the inspired research

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topics. The remainder of this paper is organized as follows: Section II summarizes the characteristics of the targeted problem and the gap for off-the-shelf methods. A simple yet effective framework, called two-stage multi-fidelity surrogate model-assisted optimization (TMSO), hybridizing MOEA and SAEA is then proposed in Section III. Section IV demonstrates and verifies TSMO using a multi-physics electro-thermo-elastic micro-actuator and a microwave dielectric resonator antenna, respectively. Section V discusses the inspired research topics when employing TSMO. The concluding remarks are provided in Section VI.

II. MOEAs and Computationally Expensive Engineering Design Optimization Problems

Engineering design optimization problems often have the following characteristics: (1) Simulation is often a must, which is computationally expensive when the required accuracy is high. (2) The objectives are often constraints themselves because of the design specifications. In addition, only the PF near the design specifications is of interest to the designer. Again taking the phase margin of an amplifier as an example, when using it as an objective, PF with performances higher than 70° or lower than 55° are redundant. (3) The designers may only need a few Pareto-optimal designs in typical locations to compare with so as to obtain the final design. A large number of Pareto-optimal designs adjacent to each other are often not essential or needed. (4) Pareto optimal may sometimes not be necessary as long as the design specifications are met.

It can be seen that characteristics (2), (3) and (4) show a subset of a conventional PF with a sufficient number of evenly distributed Pareto-optimal solutions. The requirements in completeness, distribution and quality are reduced considering these characteristics. To satisfy characteristics (2), (3) and (4), a conventional PF is obviously better but employing a conventional MOEA leads to too long optimization time due to the computationally expensive simulations. In other words, does the outcome of a conventional MOEA worth the computing efforts? To obtain a high-quality PF, the population size cannot be small (e.g., a population size of several hundred has to be used), but arguably only a few typical Pareto-optimal points are sufficient for the designer. An even distribution of the Pareto-optimal points is one of the important goals for MOEAs but it is less useful when compared against its long optimization time in real-world design practice. The importance of objective constraints is highly emphasized in engineering design optimization, but considering them only attracts attention in the MOEA field in recent years [7], [8] and no surrogate model is considered.

Owing to the above, to the best of our knowledge, there is no off-the-shelf method for the targeted engineering design optimization problem, although SAEA and MOEA have been well investigated. This asks for an alternative efficient method to address the challenge of inexact design specifications. An opportunity is to make use of the simulation models with different fidelities. Simulations models, especially those using numerical techniques (e.g., finite element analysis), are able to make a trade-off between the accuracy and the simulation time. For example, for a numerical model, when reducing the mesh density or the number of solver iterations, a less accurate but computationally much cheaper model can be obtained, which is often 2 to 50 times faster than the high-fidelity accurate model [9]. By employing the low-fidelity model, real-world designers often carry out iterative optimization. For example, the low-fidelity model is firstly used for various kinds of design specifications; knowledge is then acquired and new specifications are proposed until a potential appropriate design specification is found. The high-fidelity model will then be employed. However, this is not a systematic approach and the iterative optimization process often largely depends on the designer's experience.

In Section III, a simple yet efficient systematic framework, called TSMO, is proposed. A multiobjective optimization using a low-fidelity simulation model is firstly carried out to get a preview of the performance space. The appropriate design specifications are then obtained from the PF. A single objective surrogate-based optimization with a high-fidelity simulation model is then applied to obtain the final design. Various optimization algorithms can be employed to implement this framework. In this paper, the MOEA/D-DE method [10] and the surrogate model-aware evolutionary search (SMAS) method [11], [12] are employed for the implementation. Besides this hybrid optimization framework, a equally important contribution is that novel research topics for MOEAs and SAEAs for engineering design can be put into this framework, bridging the two domains.

III. The TMSO Framework and Its Implementation

A. The General Framework

The general framework of TMSO is shown in Fig. 1. TMSO works as follows:

Step 1: Carry out a conventional multiobjective optimization with a low-fidelity simulation model to obtain a preview of the possible optimal performance.

Step 2: Based on the information obtained from Step 1 and the assigned requirements for the building block, select the design specifications.

Step 3: Carry out surrogate model-assisted single-objective optimization to address the design specifications. A high-fidelity model is used.

Some clarifications are given below:

- The efficiency improvement of the first stage comes from the low-fidelity simulation model. This simulation model is a coarse mesh numerical model, which is often 2-50 times faster than the high-fidelity model [13].
- In the first stage, standard MOEAs, MOEAs considering objective constraints [7], surrogate-based or interactive MOEAs [5], [6] can all be employed. When the low-fidelity simulation model is computationally reasonably cheap, the first two are preferred because of higher solution quality. Otherwise, the latter two are preferred because of efficiency.

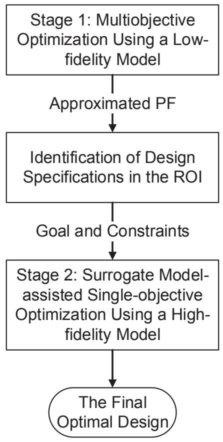

Fig. 1. The TMSO Framework.

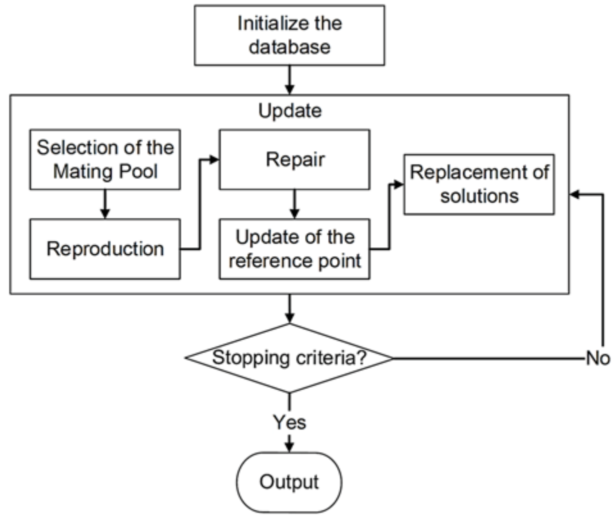

Fig. 2. The MOEAD/D-DE flow diagram.

- The low-fidelity model should still be reasonable. For example, excessively low mesh density is not recommended. The discrepancy between the low- and high-fidelity models can be observed in the initial sampling, which is a reference for the designers.
- Although the low-fidelity model is inaccurate, numerous design cases show that reasonable low-fidelity models still represent meaningful positions in the performance or objective space. It is true that for the same performance, the corresponding designs are different using simulation models of different fidelities. However, only information from the performance or objective space, instead of the design space, is used in the TMSO framework.
- The efficiency improvement of the second stage comes from surrogate model-assisted optimization techniques. Although using a high-fidelity model, the employment of surrogate models saves a number of simulations.
- SAEAs only using the high-fidelity model or making use of both low-fidelity and high-fidelity simulation data for surrogate modeling are alternatives for the second stage. When the high-fidelity simulation model is computationally very expensive, the latter is preferred. Otherwise, the former is preferred for easier implementation.

B. Implementation

It can be seen that there are several implantation methods for the TSMO framework. In the following, a conventional MOEA and an SAEA only using the high-fidelity model are selected to form the implementation.

MOEA/D-DE [10] is selected for the first stage and the flow diagram is shown in Fig. 2. MOEA/D-DE works by decomposing the approximation of the PF into N scalar optimization sub-problems using the Tchebycheff approach [**?**]. The scalar function is as follows:

$$\begin{aligned} \text{minimize} \quad & g(x|\lambda, z^*) = max\{\lambda_i|f_i(x) - z_i^*|\} \\ s.t. \quad & x \in \Omega \end{aligned} \tag{1}$$

where $\lambda = (\lambda_1, ..., \lambda_m)$ is a weight vector and $\sum_{i=1}^{m} \lambda_i = 1$, Ω is the solution space and $z^* = (z_1^*, ..., z_m^*)$ is the reference point. If N is reasonably large, the optimal solutions to the scalar functions yield a very good approximation to the PF.

Differential Evolution (DE) [14] is the search engine in MOEA/D-DE. If P is a population having $x = (x_1, \ldots, x_d) \in R^d$ as an individual solution in it, DE creates a child solution $c = (c_1, \ldots, c_d)$ for x by producing a donor vector via mutation and carrying out crossover operations on it [14]. More details can be found in [14].

As shown in Fig. 2, after initialization, in each iteration of MOEA/D-DE, the mating pool is randomly selected and reproduction is carried out using DE operators and polynomial mutation to generate new solutions. Solutions out of the bounds of Ω in (1) are repaired, updated and replaced. If a stopping criterion is met, a PF of design solutions is generated as the output.

The optimizer of the second stage is the surrogate model-aware evolutionary search (SMAS) method [11], [12] and the flow diagram is shown in Fig. 3. In SMAS, DE is also the global search engine and Gaussian process is used for surrogate modelling [15]. SMAS carries out single-objective optimization and comparisons show its advantages over several popular SAEAs [11], [12].

As shown in Fig. 3, following a small number of initial samples, in each iteration, a fixed number (k) of top-ranked candidate solutions are used to generate new solutions by applying DE operators. Surrogate models are then constructed using the nearest number (τ) of training data points in the search space. The new child solutions are prescreened using the lower confidence bound method [16] and numerical simulation is carried out only on the best solution, i.e., the top 1 individual. More details can be found in [11], [12].

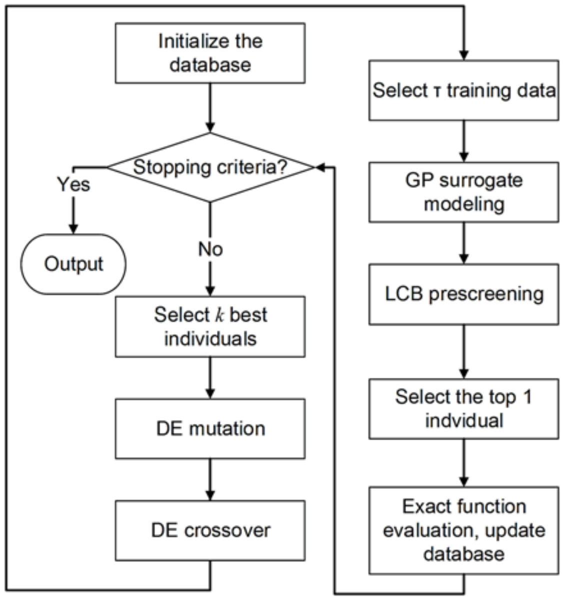

Fig. 3. The SMAS flow diagram.

IV. Real-world Design Cases

In this section, two real-world engineering design problems are used to demonstrate the TSMO framework. The first problem is the design and optimization of the four-variable multi-physics electro-thermo-elastic micro-actuator [17] and the second problem is the design and optimization of the seven-variable hybrid dielectric resonator antenna [18]. For both problems, the implementation of TSMO is according to Section II. The parameter settings for MOEA/D-DE are the same for all experiments: a population size of 100 is used and other algorithmic settings are based on the recommendations in [10]. For the SMAS method, all the parameter setting rules are the same for all experiments and are based on the recommendations in [11], [12]. All experiments are carried out on a workstation with an Intel 4-core i7-4770 3.50 GHz CPU and a 24 GB RAM and the time consumption reported is wall clock time.

A. Case 1: Multi-physics Electro-thermo-elastic Micro-actuator

The first design case is a multi-physics electro-thermo-elastic micro-actuator and the layout is shown in Fig. 4. It is modeled in COMSOL Multiphysics according to the forward problem in [17]. Its parametric 3-D finite-element model has a typical mesh composed of about 5,000 and 40,000 3-D elements for the low-fidelity and high-fidelity models, respectively. Each low-fidelity simulation costs 15 to 40 seconds and each high-fidelity simulation costs 4 to 10 minutes on the adopted workstation.

The micro-actuator is a part of a sensor, which follows a top-down design flow. The coarse specifications assigned are as follows: the maximum temperature (T_{max}) should be at most $450K$, but if T_{max} can reach $430K$, it is preferred; the total displacement (u) should be around $2\mu m$, but a larger value such as $2.1\mu m$ is preferable; the stress (S) must be smaller than $1.44GPa$. Considering all these, the size of the micro-actuator should be as small as possible.

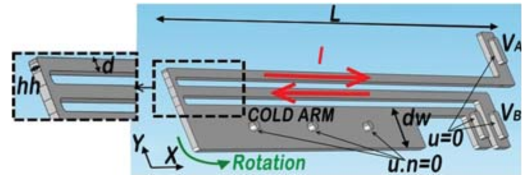

Fig. 4. Geometry and design variables of the micro-actuator.

TABLE I
Ranges of the design variables for the design exploration of the micro-actuator (all sizes in μm)

$Variables$	l	hh	dw	d
Lower bound	56	2	7	1
Upper bound	300	5	30	7

The optimization goal is to find optimal values for the following design variables, as shown in Fig. 4: L (length of the actuator), hh (thickness of the actuator), dw (width of the cold arm) and d (width of the hot arms). For the design exploration, the search boundaries are shown in Table I. The TMSO framework is then employed.

In the first stage, a multi-objective optimization problem (Problem 1) is defined to preview the feasibility of the anticipated design requirements; find a set of solutions that simultaneously minimizes the maximum temperature (T_{max}) and maximizes the total displacement (u), subject to the following constraints:

$$\text{Geometric congruency: } dw < 2 \times d \tag{2}$$

$$S < 1.44\ GPa \tag{3}$$

Fig. 5 shows the approximated PF obtained (using the low-fidelity simulation model) after 79 iterations (7900 low-fidelity simulations, 45.5 hours). From the approximated PF found by solving Problem 1 using MOEA/D-DE, the designer selects one non-dominated solution (T_{max-ND}, u_{ND}), where T_{max-ND} and u_{ND} are the real specifications identified and selected to be: $T_{max-ND} = 435K$ and $u_{ND} = 2.1\mu m$.

Using the selected specifications from the outcome of the first stage, the second stage is a single-objective optimization (Problem 2) solved by using the SMAS method with the high-fidelity model of the micro-actuator. The aim of this stage of the optimization is to find the optimal solution, which minimizes the micro-actuator area (A) defined by:

$$\begin{aligned} &\text{minimize} \quad A = L \times (dw + 2 \times d) \\ &s.t. \\ &\quad T < T_{max-ND} \\ &\quad u > u_{ND} \\ &\quad S < 1.44\ GPa \end{aligned} \tag{4}$$

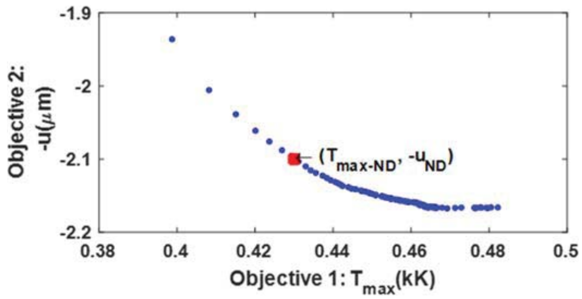

Fig. 5. Pareto front of the multi-objective optimization (Stage 1) for example 1.

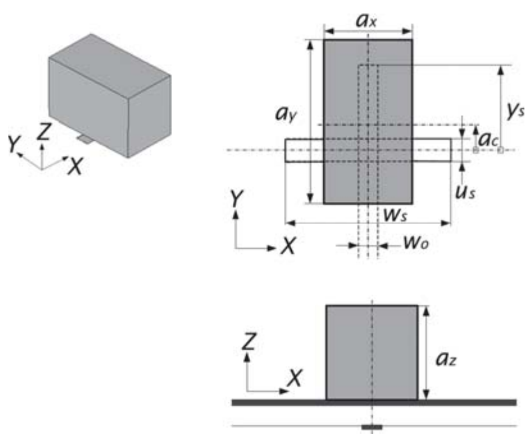

Fig. 6. Layout and design variables of the hybrid dielectric resonator antenna.

The ensuing single-objective optimization obtains a design geometry that satisfies all the constraints after 122 simulations (7.7 hours). It then converges after 370 simulations (40.5 hours) to obtain a micro-actuator area of $9.46nm^2$, $T_{max} = 433.9K$, $u = 2.1\mu m$ and $S = 0.251GPa$. Note that a satisfactory design is obtained after about 140 simulations (16 hours) with $9.6nm^2$. The final micro-actuator design has the following geometry: $L = 300\,\mu m$, $hh = 5\,\mu m$, $dw = 8.1\,\mu m$ and $d = 1.73\,\mu m$. The total design time is 86 hours.

MOEA/D-DE with the high-fidelity model is also employed for comparison. After 86 hours, the latest PF is still far from optimal. Note that the PF in Fig. 3 is formed after 7900 low-fidelity simulations and the use of high-fidelity simulations is about 15 times slower. Thus, generating a PF with a conventional MOEA with the high-fidelity model directly could be prohibitive.

B. Case 2: Hybrid Dielectric Resonator Antenna

The second case is the hybrid dielectric resonator antenna (DRA) [18] and the layout is shown in Fig. 6. The hybrid DRA is modeled and discretized in Computer Simulation Technology - Microwave Studio using the time domain finite integration technique method with an accuracy of -30 dB. Mesh densities of 10 cells per wavelength (resulting in about 16,000 hexahedral mesh cells) and 30 cells per wavelength (resulting in about 162,000 hexahedral mesh cells) are used for the low-fidelity and high-fidelity models, respectively. Each low-fidelity simulation costs 10 to 30 seconds and each high-fidelity simulation costs 1 to 5 minutes on the adopted workstation.

TABLE II
RANGES OF THE DESIGN VARIABLES (ALL SIZES IN MM) FOR HYBRID DRA DESIGN EXPLORATION

$Variables$	a_x	a_y	a_z	a_c	u_s	w_s	y_s
Lower bound	6	12	6	6	0.5	4	2
Upper bound	10	16	10	8	4	12	12

The hybrid DRA is implemented on a RO4003C substrate using a relative permittivity (ϵ_r) of 3.38, a loss tangent (tan(δ)) of 0.0027 and a thickness of 0.5 mm. The excitation is via aperture coupling with $TE_{\delta 11}$ mode. The excitation mode, coupling, and resonances of the hybrid DRA are all influenced by its physical dimensions [19]. As shown in Table II and Fig. 6, the dimensions of the DR brick (a_x, a_y and a_z) and slot (u_s and w_s), the length of the microstrip slab(y_s), and the location of the DR relative to slot (a_c) are the critical design parameters for the design exploration. A geometric constraint ($a_c \leq 0.5 \times a_y$) is used to ensure the slot remains under the DRA in all possible cases during the optimization.

For a typical wideband wireless LAN (WLAN) application using the hybrid DRA [20], a design solution providing a maximum in-band S_{11} of around -20 dB and a minimum in-band G_R of around 4 dBi is sufficient. Optimal design solutions with a lower value for the maximum in-band S_{11} (e.g., -21 dB) is not necessary. This is because a return loss of -20 dB means 99% of the signals are received. For the minimum in-band G_R, lower or higher values may be required (especially in the hybrid DRA's boresight) depending on the application [21]. In practice, a value of around 4 dBi for the minimum in-band G_R is essential for 5-GHz WLAN application [20].

As explained above, considering a WLAN application for the hybrid DRA in the wideband 5.28 GHz to 5.72 GHz for this example, the designer is not certain to what extent the hybrid DRA will be able to meet the specifications for S_{11} and G_R in the bandwidth. As a result, using a low-fidelity model, the performance or objective space of the hybrid DRA is firstly explored inexpensively to identify the feasible performance region for both S_{11} and G_R. This constitutes a multi-objective optimization problem which aims to find a set of solutions that satisfies the goals in (5) and (6) at the first stage.

$$\text{minimize}\ \ max(S_{11})\ \ 5.28\,GHz - 5.72\,GHz \tag{5}$$

$$\text{maximize}\ \ min(G_R)\ \ 5.28\,GHz - 5.72\,GHz \tag{6}$$

After 2764 low-fidelity EM simulations in a total of 21 hours, a design solution is found on the current PF which is yet to converge: $max(S_{11})_{ND}$ = -20.6 dB and $min(G_R)_{ND}$ = 4.1 dBi in the frequency bandwidth. Although it is not yet the final Pareto optimal design, sufficient information is available

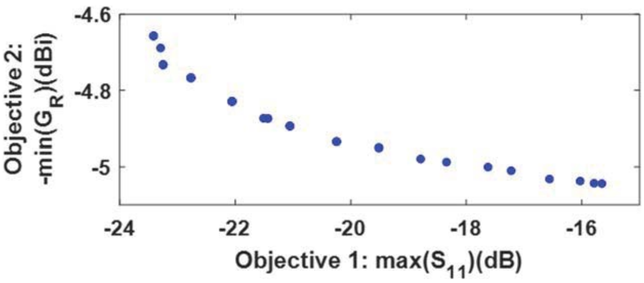

Fig. 7. Pareto front of the multi-objective optimization (Stage 1) for example 2.

for the second stage. The approximated PF after 300 iterations (30000 low-fidelity simulations, 240 hours) is also shown in Fig. 7. It can be seen that although more improvements can be made, it is not necessary for this design case.

Using the reference values from the first stage, the second stage is a single-objective optimization addressed by using the SMAS method with the fine or high-fidelity model of the hybrid DRA. The aim is to find an optimal design solution, which provides the maximum possible in-band $min(G_R)$ subject to an in-band $max(S_{11})$ of not more than -20 dB (inferred from the approximated PF) as stated in (7). A penalty coefficient of 50 is used to ensure that the optimization focuses on meeting the $max(S_{11})$ specification first and upon satisfying the constraint on $max(S_{11})$. The stopping criterion is $min(G_R) \geq 4.0$ dBi in consonance with the intended application.

$$\begin{aligned} &\text{maximize} \quad min(G_R) \;\; 5.28\,GHz - 5.72\,GHz \\ &s.t. \\ &\quad max(S_{11}) \leq -20\,dB \;\; 5.28\,GHz - 5.72\,GHz \end{aligned} \tag{7}$$

After 390 high-fidelity simulations in a total of 18 hours, the SMAS method obtains a design solution with the following performance specifications: $max(S_{11})$ = -20.3 dB and $min(G_R)$ = 4.7 dBi. The final hydrid DRA design has the following geometry: $a_x = 6.62\,mm$, $a_y = 14.88\,mm$, $a_z = 9.98\,mm$, $a_c = 3.57\,mm$, $u_s = 0.71\,mm$, $w_s = 8.76\,mm$ and $y_s = 2.95\,mm$. The total design time is 39 hours.

A comparison is not made for the case of using MOEA/D-DE with the high-fidelity model of the hybrid DRA. This is because the computational cost (which is estimated to more than 3 months and about 10 times slower) is not affordable.

V. New Research Topics Inspired from TSMO

The above section shows that the two-stage structure of TSMO is suitable for efficient real-world engineering design optimization. Stage 1 carries out a multiobjective optimization employing relatively cheap low-fidelity models to investigate the feasibility and trade-off among the intended design specifications. Informed by the first stage, the second stage carries out surrogate model-assisted single-objective optimization employing an accurate expensive high-fidelity model.

Novel MOEAs and SAEAs for engineering design can be investigated either for Stage 1 or Stage 2 bridging the two domains, some of which are listed as follows:

- In Stage 1, although the low-fidelity model is employed making a conventional MOEA finish in a practical time-frame, the PF generated by conventional MOEAs is still redundant. This is because only a small part of the PF near the intended design specifications is useful. Therefore, novel MOEAs which quickly concentrates on the interested small part is of particular importance.
- For some design cases, the low-fidelity model is not computationally cheap. This inspires the research of introducing surrogate models to the last item. Note that this is different from existing surrogate model-assisted MOEAs, because only a small part of PF near the specifications is the focus.
- Conventional MOEAs often need a sufficient population size to obtain a good-quality PF, but the many points in the PF are not essential or even necessary from the engineering design point of view. When even the low-fidelity model is computationally expensive, MOEAs which use a small population size to obtain a high-quality PF are of particular interest.
- For some design cases, the specifications that are being traded-off could be up to 10. Many-objective MOEAs considering the above three items become an interesting research topic.
- Besides supporting the determination of appropriate design specifications for the second stage, the low-fidelity simulations provide information about the design landscape characteristics for the design problem. SAEAs which make use of the information from low-fidelity simulations to support Stage 2 is useful when the high-fidelity model is computationally very expensive.

VI. Conclusions

In this paper, solutions for computationally expensive engineering design optimization problems without exact design specifications are investigated. The characteristics of the targeted problem are firstly summarized; the gap between off-the-shelf MOAEs and SAEAs and the practical need is then analyzed. A simple yet effective framework, called TSMO, is proposed to improve efficiency and its suitability is demonstrated by two real-world design cases. The research topics inspired by the TSMO framework are presented aiming to generate new MOAEs and SAEAs particularly for engineering design optimization.

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