



Issues in Deciding Whether to Use Multifidelity Surrogates

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Multifidelity surrogates are essential in cases where it is not affordable to have more than a few high-fidelity samples, but it is affordable to have as many low-fidelity samples as needed. In these cases, given a good correlation between the models, the performance of multifidelity models can be outstanding. The first objective of this paper is to discuss progress in creating accurate multifidelity surrogates when they are essential. A more ambiguous situation exists when it may be possible to afford enough high-fidelity samples to construct an accurate surrogate model. In that case, the question is whether a multifidelity surrogate will afford a substantial cost reduction for comparable accuracy. Our second objective is to see if there are any indications under what circumstances this substantial cost reduction is realized. From the literature, it appears that it is hard to get an idea, in terms of cost savings, of when it is useful to invest the additional effort of creating and using multifidelity surrogates. It is observed that in some cases the inclusion of low-fidelity samples along with the high-fidelity samples in building multifidelity surrogates led to less accurate surrogates than just using the available high-fidelity samples.

Nomenclature

$y_{HF}(\mathbf{x})$	=	high-fidelity model
$\hat{y}_{HF}(\mathbf{x})$	=	high-fidelity surrogate
$y_{LF}(\mathbf{x})$	=	low-fidelity model
$\hat{y}_{LF}(\mathbf{x})$	=	low-fidelity surrogate
$\hat{y}_{MF}(\mathbf{x})$	=	multifidelity surrogate
$\delta(\mathbf{x})$	=	discrepancy function
$\hat{\delta}(\mathbf{x})$	=	discrepancy function surrogate, also known as additive correction
$\mu(\mathbf{x})$	=	multiplicative function
$\hat{\mu}(\mathbf{x})$	=	multiplicative function surrogate, also known as multiplicative correction
ρ	=	constant scaling factor

I. Introduction

SURROGATES are approximations often built to reduce computational cost when a large number of expensive simulations are needed for such processes as optimization (e.g., [1] or [2]) and uncertainty quantification (e.g., [3]). The data used to construct surrogates come from models. To refer to the value of the design variables and the corresponding response obtained from a model, in this work, we use data, data points, and samples interchangeably. Models refer to physical models used to describe the physics of the studied phenomenon as in the case of computational fluid dynamics (CFD), direct numerical simulation (DNS), large-eddy simulation (LES), Timoshenko beam theory, established algebraic models, experiments, and so on. However, when it comes to surrogates, no matter how complex the physics are, the quantity of interest is approximated using algebraic functions of the variables of interest. Therefore, the complexity of the physics is involved in the function evaluation, but the quantity of interest is assumed to be a smooth function of the design variables. For example, in the case of turbulent

flows, the response is chaotic, but the average flow velocity over a channel can be approximated as a smooth function of the channel size.

High-fidelity (HF) models usually represent the behavior of a system to acceptable accuracy for the application intended. These models are usually expensive, and their multiple realizations often cannot be afforded, for example, in fluid mechanics a highly refined grid Reynolds-averaged Navier–Stokes (RANS) (e.g., [4]) or DNS (e.g., [5]). On the other hand, low-fidelity (LF) models are cheaper but less accurate. Examples of LF models in the context of multifidelity (MF) are dimensionality reduction (e.g., [6]), simpler physics models (e.g., [7]), coarser discretization (e.g., [8,9]), and partially converged results (e.g., [10]). Whether a model is LF or HF is problem dependent, and it can be decided based on the cost and accuracy against other fidelities available, which depend on the accuracy being sought. The surrogate model constructed using data from the chosen LF model is called LF surrogate. Similarly, a surrogate built using HF data is called HF surrogate. While a single-fidelity surrogate is an approximation built using data coming from a single model (experimental data can be also considered), MF surrogates combine the information of multiple models, with different cost and accuracy (fidelity). MF surrogates have drawn much attention in the last two decades because they hold the promise of achieving the desired accuracy at a lower cost.

In this paper, we will mainly focus on MF surrogates, that is, surrogates built with data from both LF and HF models. However, MF hierarchical methods can also be found in the literature. MF hierarchical methods are approaches that use LF and HF models/surrogates following a criterion (e.g., in optimization, using LF model/surrogate for computation until finding the optimum, then the HF model/surrogate is used to increase the accuracy in finding the extrema). In this work, we refer to MF methods and MF approaches interchangeably. MF methods encompass both MF surrogates and MF hierarchical methods.

In this paper, we investigate the usefulness of MF surrogates in the perspective of cost savings and accuracy improvement. We first consider the case when MF surrogates are essential, because we cannot afford the cost of enough HF simulations to construct an HF surrogate of acceptable accuracy. Here our objective is to discuss recent progress in MF construction for improving MF surrogate accuracy. Then we consider the case when we may be able to afford enough HF simulations for an acceptably accurate HF surrogate, but an MF surrogate may offer superior accuracy at comparable cost. MF surrogates often require an investment of time and effort for implementation. Here our objective is to probe the literature as to when the payoff justifies the effort. There is the additional question of whether MF surrogates should be constructed even if no effort is required. As [11] and [12] have shown, at times using the LF samples leads to a surrogate that is less accurate than the one using only HF samples. We look for indications as to when this may happen.

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This paper is organized as follows. In Sec. II we briefly describe the surrogates most used in the context of MF. There are multiple surrogates available and the best choice will strongly depend on the characteristics of the problem. In Sec. III we show that substantial progress has been achieved in the past few years in the accuracy of MF surrogates by combining additive and multiplicative corrections. Earlier MF surrogates typically used only one or the other. Recent work combines both corrections and we attempt to clarify the benefit of this combination. In Sec. IV we summarize the findings in some recent papers, discussing the following issues:

1) How can we decide when to use only the HF samples to construct a surrogate rather than fusing together the HF and the LF samples in an MF surrogate?

2) If we decided to build an MF surrogate, how can we choose between multiple LF models?

3) How to use both additive and multiplicative factors in MF for surrogates other than the ones that use Gaussian process?

Section V discusses cost-savings issues in MF surrogates, and it is divided in two sections. In Sec. V.A we survey papers that provide the cost of an optimization done using an HF surrogate and an optimization done using an MF surrogate for optimizing the same physical problem. We hypothesized that the cost savings resulting from using MF surrogates might be related to the cost ratio between the HF models and the LF models. If the LF model is very cheap compared with the HF model but they are well correlated, we can expect for the MF surrogate to do a good job at a lower cost.[†] We plot the relative optimization cost as a function of the relative fidelities cost and we discuss our findings. Based on the extensive review of papers employing MF surrogates, it was found that usually the literature reports the success of using MF surrogates but rarely discusses the cause of the success. This is in spite of substantial progress in the accuracy of MF approaches. In Sec. V.B we suggest guidelines for reporting computational cost-effectiveness by using MF surrogates. Because cost saving is of great interest to many different fields, reporting it would help other researchers in deciding whether or not to use MF surrogates in their applications. In Sec. VI we include recommendations based on our experience that can help users to get the most out of MF surrogates under certain conditions. In addition, we included two appendices. Appendix A discusses different techniques for design of experiment in MF surrogates context. Appendix B shows statistics extracted from reviewing extensive literature in MF approaches.

II. Surrogates

Most surrogates are algebraic models that approximate the response of a system based on fitting a limited set of computationally expensive simulations in order to predict a quantity of interest. Surrogates are widely used while constructing MF methods. The information of different types of fidelities can be included in a single surrogate through an MF surrogate (e.g., in [13–15]). Alternatively, surrogates can be constructed for each fidelity separately and never combined explicitly in an MF surrogate. These are called MF hierarchical methods (e.g., in [16,17]). Here the MF method is the efficient way that these surrogates are constructed and/or applied in order to obtain significant savings.

The accuracy of a surrogate is determined by the complexity of the function, by the design of experiment used to select the data points, the size of the domain of interest, the simulation accuracy at the data points, and the number of samples available [18]. Reference [19] included a complete section of projection-based models and data-fit models where the reader can extend the information included in this section.

Response surface surrogates are the oldest and they may still be the most widely used form of surrogates in engineering design. Response

surface surrogates are fitted by linear regression combining simplicity and low cost as it only requires the solution of a set of linear algebraic equations. Response surface usually assumes that the functional behavior (e.g., a second-order polynomial) is correct, but the response has noise. In the MF context, response surface can be found in a large number of papers—to cite some of them, [20–36].

Polynomial chaos expansion became popular in this century for the analysis of aleatory uncertainties using probabilistic methods in uncertainty quantification [37–39]. In polynomial chaos expansion, the statistics of the outputs is approximated by constructing a polynomial function that maps the uncertain inputs to the outputs of interest. The chaos coefficients are estimated by projecting the system onto a set of basis functions (Hermite, Legendre, Jacobi, etc.). In MF context, polynomial chaos expansion applications can be found, for example, in [3,15,40–42].

With increasing computer power, more expensive surrogates became popular. These include kriging, artificial neural networks, moving least squares, and support vector regression. These usually work better for highly nonlinear, multimodal functions.

Kriging surrogate estimates the value of a function as the sum of a trend function (e.g., polynomial) representing low-frequency variation, and a systematic departure representing high-frequency variation components [43]. Unlike response surface, most kriging approaches assume that the response is correct but the functional behavior is uncertain. Kriging has become a very popular surrogate in general, but even more so for MF applications. This may reflect the fact that it has an uncertainty structure that lends itself to nondeterministic MF methods. Applications of kriging surrogates in the MF context can be found in [1,44–47].

Co-kriging [48,49] is commonly known as the extension of kriging to include multiple levels of fidelities in the surrogate construction. Applications of co-kriging can be found in [50–53]. Reference [54] compared kriging and co-kriging performance.

Artificial neural networks consist of artificial neurons that compute a weighted sum of inputs and pass it through a saturation function to compute the output of the artificial neuron. An example of artificial neural networks application in MF approaches can be found in [7], where it is used during the optimization process to correct the aerodynamic forces in the simplified LF model using a CFD HF model. The LF model is used to generate samples globally over the range of the design parameters, whereas the HF model is used to locally refine the artificial neural networks surrogate in later stages of the optimization.

Another well-known surrogate is moving least squares, which was introduced by [55] and was extensively discussed in [56]. Moving least squares is an improvement of weighted least-squares (proposed by [57]). Weighted least-squares recognizes that all design points may not be equally important in estimating the polynomial coefficients. A weighted least-squares surrogate is still a straightforward polynomial, but with the fit biased toward points with a higher weighting. In a moving least squares surrogate, the weightings are varied depending upon the distance between the point to be predicted and each observed data point. Examples of its implementation in MF can be seen in [58–62].

Traditional surrogates predict scalar responses. Some nontraditional ones, such as proper orthogonal decomposition, are used to obtain the entire solution field to a partial differential equation. References [63–65] explore the MF proper orthogonal decomposition method in fluid mechanics.

III. Progress in Fitting Surrogates to Given Data

We first consider the case where MF surrogates are a must because we cannot afford enough simulations to obtain an HF surrogate of acceptable accuracy. Here great progress was achieved in this century in improving the accuracy of MF surrogates using only a small number of HF simulations.

MF surrogates are built using more than one fidelity. Early MF surrogates mostly used additive or multiplicative corrections (e.g., [10,23,66]). Given an LF model, $y_{LF}(\mathbf{x})$, and an HF model, $y_{HF}(\mathbf{x})$, we denote their surrogates as $\hat{y}_{LF}(\mathbf{x})$ and $\hat{y}_{HF}(\mathbf{x})$, respectively.

[†]Optimization usually needs a large number of iterations. In each optimization iteration, a single analysis is performed. This analysis might come from the actual model (RANS, DNS, Euler, etc.) or from the surrogate approximation of these models. On top of this, the surrogates can be constructed using HF data points, LF data points, or both (MF surrogates).

In general, we use $\hat{\cdot}$ to denote a surrogate model. The additive correction approach assumes that the relation between $y_{LF}(x)$ and $y_{HF}(x)$ is additive; therefore, we can write

$$\hat{y}_{MF}(x) = \hat{y}_{LF}(x) + \hat{\delta}(x) \tag{1}$$

where $\hat{\delta}(x)$ is the surrogate constructed using the difference between the $y_{HF}(x)$ and $y_{LF}(x)$ models at nested data points (i.e., data points where we have both LF and HF model computations) and $\hat{y}_{LF}(x)$ is the LF surrogate constructed with samples from the LF model, $y_{LF}(x)$. If the LF model is cheap enough (e.g., an algebraic approximation), we can use the simulations directly without constructing the LF surrogate \hat{y}_{LF} . In this case, Eq. (1) becomes

$$\hat{y}_{MF}(x) = y_{LF}(x) + \hat{\delta}(x) \tag{2}$$

The decision whether to use directly the LF function or replace it with a surrogate depends on its cost, complexity, and the number of needed surrogate evaluations. In some applications (e.g., [26]) the LF function is very cheap, and so replacing it with a surrogate leads to unnecessary loss of accuracy. In others, the number of simulations needed for constructing an accurate surrogate to the LF function is very high. For example, in [67] even thousands of LF simulations did not suffice for an accurate LF surrogate. If the number of LF data available is higher than the number of needed evaluations of the surrogate (e.g., for optimization), then it may be better not to replace the LF function by a surrogate.

The multiplicative approach is

$$\hat{y}_{MF}(x) = \hat{\mu}(x)\hat{y}_{LF}(x) \tag{3}$$

where $\hat{\mu}(x)$ is the surrogate constructed using the quotient between $y_{HF}(x)$ and $y_{LF}(x)$ models at the nested data points. Similarly if the LF model is very cheap enough, there is no need to construct $\hat{y}_{MF}(x)$; therefore, Eq. (4) becomes

$$\hat{y}_{MF}(x) = \hat{\mu}(x)y_{LF}(x) \tag{4}$$

A substantial improvement in accuracy was achieved by the introduction of a scalar multiplier to the LF function (e.g., [68,69]). The following form of MF surrogates is called the comprehensive approach. For the comprehensive approach, additive and multiplicative corrections are combined

$$\hat{y}_{MF}(x) = \rho\hat{y}_{LF}(x) + \hat{\delta}(x) \tag{5}$$

where ρ is a constant. In this formulation, $\hat{\delta}(x)$ is usually called the discrepancy function. Again, if the LF model is cheap enough, we might consider the use of LF simulations instead of the LF surrogate. In this case, Eq. (5) becomes

$$\hat{y}_{MF}(x) = \rho y_{LF}(x) + \hat{\delta}(x) \tag{6}$$

MF surrogates are called for when we have a complicated function, and 1) we cannot afford enough samples to construct a surrogate that would capture the complexity of the function, and 2) we have a cheap LF function with a similar behavior. The ideal situation for an MF surrogate is when the difference between the HF function and a scaled LF function has a simple behavior that can be captured by a surrogate fitted to small number of samples. Consider, for example, an HF model, y_{HF} ,

$$y_{HF}(x) = \sin(20x) + x, \quad 0 \leq x \leq 1 \tag{7}$$

and an LF model, $y_{LF}(x)$,

$$y_{LF}(x) = \sin(20x) + 0.5x + 0.5, \quad 0 \leq x \leq 1 \tag{8}$$

where $x \in \mathbb{R}$.

If we cannot afford more than two or three HF samples but we can afford a very large LF number of samples, the MF surrogate with

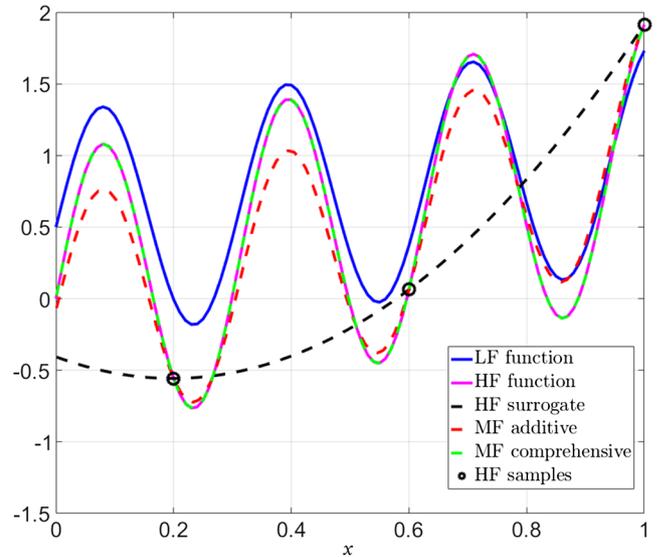


Fig. 1 The HF and LF functions [Eqs. (7) and (10), continuous lines] along with the three approximations constructed (dashed lines). The MF comprehensive surrogate predicts the HF function exactly.

additive correction will give as a perfect fit because the discrepancy function can be calculated exactly as follows:

$$\hat{\delta}(x) = -0.5x - 0.5 \tag{9}$$

Often, however, the complex part requires some scaling. For example, consider that instead of Eq. (8) we have an LF model, $y_{LF}(x)$, as follows

$$y_{LF}(x) = 0.8 \sin(20x) + 0.5x + 0.5, \quad 0 \leq x \leq 1 \tag{10}$$

where $x \in \mathbb{R}$. Then an additive correction will not do the job, because the difference between the two functions is $0.2 \sin(20x) - 0.5x - 0.5$, and this cannot be fitted by an accurate surrogate with only two or three samples of the difference. However, a comprehensive MF surrogate will do the trick, by using $\rho = 1.25$ and $\hat{\delta}(x) = 0.375x - 0.625$. Let assume that we can afford 3 HF samples at $x_1 = 0.2$, $x_2 = 0.6$, $x_3 = 1.0$. Using linear regression with monomial basis functions up to second order, we obtain the results shown in Fig. 1 and Table 1.

Table 1 shows that this is a clear example where MF surrogates will work very well. Note that even the MF additive correction does a decent job and greatly improves on the HF surrogate performance.

References [70,71] looked at the success of the combination of Gaussian process or kriging surrogates with a Bayesian identification of ρ and $\hat{\delta}(x)$ by using the maximum likelihood estimation. They concluded that the Bayesian approach tends to minimize the bumpiness of $\hat{\delta}(x)$ so that it can be fitted accurately with a small number of available HF samples. In other words, we improve the correlation between HF and LF models by minimizing the bumpiness. In one dimension the bumpiness b of a function $f(x)$ is defined as the integral of the square of the second derivative as

$$b = \int |f''(x)|^2 dx \tag{11}$$

Table 1 Correction functions and RMSE errors obtained for each surrogate constructed

Surrogate	ρ	$\hat{\delta}(x)$	RMSE
HF	—	$-0.406 - 1.523x - 3.482x^2$	0.9565
MF additive	—	$-0.581 - 0.005x + 0.768x^2$	0.1913
MF comprehensive	1.25	$-0.625 + 0.375x$	0

In higher dimensions, Ref. [71] averaged the bumpiness over a large number of lines in random directions. For the examples that they examined, the minimum error was very close in value to the one that minimizes bumpiness.

IV. Challenges in Fitting Multifidelity Surrogates

Sometimes we do not have any choice, and MF surrogates are the only option, for example, if we can afford only one or two samples of the HF model. However, sometimes we do have the option of choosing between building a surrogate using just the HF samples or combining HF and LF samples. We found that it is not clear when to do this and the following sections illustrate this fact.

A. Deciding Whether to Use the Low-Fidelity Data

It is not given that MF surrogates will always lead to better accuracy than a surrogate using only the HF data. As recently reported by [11], in a strength prediction problem, unexpectedly the surrogate built using only 3 or more HF samples was found to have better accuracy than an MF surrogate with the same 3 samples, aided by 12 LF samples in a two-dimensional problem. This means that, given HF and LF samples, we need a criterion to decide whether to use the LF samples with an MF surrogate or to fit a surrogate to the given HF data only.

Using the comprehensive correction with ρ in Eq. (5), it appears as if the maximum-likelihood estimation could select $\rho = 0$, which would correspond to disregarding the LF data. However, Ref. [12] tested the maximum-likelihood estimation for a two-design-variable turbine problem with a single HF model and two alternative LF models. Here, two unsteady RANS equation solvers were used: a full transient model (HF model), a transient rotor blade model with time transformation (LF model 1, LF1), and a steady RANS solver (LF model 2, LF2). The main difference between steady-state and transient models was their settings of the interface between stator and rotor. The difference between the two transient models was the turbulence model. The shear stress transportation coupled by transition is not available in the LF1 model; therefore its accuracy would be poorer than the HF model. They varied the number of HF samples ranging from 4 to 12 with 20 different designs of experiments for each number of even samples. Therefore, a total of 100 sets of design of experiments were conducted. For each case, 36 LF samples were used. The LF samples were available at a 6×6 grid, which precluded using the more common MF surrogate designs of experiments described in Appendix A. The MF surrogate was more accurate than the HF surrogate for 59 of the 100 for the better LF model (LF1), and for 18 out of 100 for the poorer LF model (LF2). However, the maximum-likelihood correctly selected $\rho = 0$ for only 3 of the 123 cases (41 cases when using LF1 and 82 when using LF2) where the HF model was more accurate. Reference [12] also tested cross-validation for the same purpose. Cross-validation was able to identify 67 of these 123 cases.

An analysis of the failures discussed in the previous paragraph indicated that the bumpiness of the correction was substantially lower than that of the HF function, because of its lower range of variation. This predisposed both the maximum-likelihood and cross-validation estimation in favor of the MF surrogate. Therefore, the maximum-likelihood and cross-validation estimations were not accurate to determine whether LF data were useful or not.

Thus, it appears that we may still lack a dependable criterion to tell whether we gain by using the LF data. Of course, there are many cases where the MF surrogate should be clearly more accurate, as, for example, most of the cases when we have only a single HF sample. However, more research into the choice between HF-alone surrogate and MF surrogate is clearly called for.

B. Choosing Between Multiple Low-Fidelity Datasets

When there are multiple LF models available, several options are possible: using all LF models, using only a subset of LF models, using the best LF model, or not using any LF model. This challenge is related to the previous challenge of deciding whether to use the LF data points available. The study by Ref. [12] indicated a possible

problem in choosing between two LF surrogates for an MF surrogate. In their study, LF1 was more useful than LF2 because it had a better correlation with the HF data so that the discrepancy function had a significantly lower range of variation (Sec. III). Out of 100 sets of designs of experiments, the MF surrogates based on LF1 surrogate were more accurate than the MF surrogates based on LF2 85 times. Cross-validation identified 71 of these cases, whereas maximum-likelihood 81. In addition, the maximum-likelihood estimation could not identify a single case of the 15 exceptional cases, and the cross-validation estimation only 6 out of the 15. This study indicated that the performance of MF surrogate depends on the design of experiments in addition to the quality of LF models. Moreover, maximum-likelihood and cross-validation estimations were not good at choosing a better LF model for a given design of experiments. This one example is not necessarily a proof that the difficulty is common. However, it is an indication that the choice between multiple LF models may be a challenge deserving of more research. Another option is to use all available LF models in a single MF surrogate as in [72,73]).

C. Selecting ρ for Other Surrogates

In Sec. III, it was shown that introducing the scaling factor ρ significantly improved the performance of MF surrogates, by reducing the bumpiness in the additive correction. The constant scaling factor ρ can be found by minimizing the bumpiness of the additive correction or by minimizing the error between the scaled LF predictions with that of HF samples. Reference [70] showed that the former performs better than the latter because it is efficient to fit a simple additive correction with a small number of HF samples. They also observed that maximizing the likelihood function in Gaussian process surrogates is similar to reducing the bumpiness in the additive correction. However, the MF surrogates using Gaussian process surrogates require uncertainty model for prediction—not all surrogates provide one.

While kriging or Gaussian process surrogates are often the most accurate or at least close to the most accurate, there are cases when other surrogates are more accurate (e.g., [74]). In particular, kriging does not work well with a very noisy response or with a very large number of samples, especially when some of them are tightly clustered. When nonkriging surrogates are used for constructing the LF surrogate and the additive correction, it is unclear how the bumpiness can be reduced effectively. One may use a kriging model for obtaining ρ but then switch to a different surrogate for fitting the MF surrogate. This approach may deserve further study. In addition, it is possible to treat the LF model as a basis with the scaling factor ρ as an unknown coefficient in linear regression. This was suggested by [69], and implemented successfully in [67].

V. Cost Ratio Versus Savings

A. Evidence from Literature

We examined the efficacy of MF surrogates for cost and time savings while maintaining the desired accuracy. Because cost and time savings are the main goal of using MF, it would be appropriate for researchers to report in their publications the cost savings by using MF surrogates. We were able to collect, from some publications that used MF surrogates for optimization, the cost ratio between performing a single analysis of LF and HF, and the cost ratio between performing optimization using MF surrogates and using HF surrogates.

Optimization processes such as genetic algorithms or gradient-based methods consist in multiple iterations until converging to the predicted optimum. In each of these iterations, there is a computation of the model used or their surrogate. Usually, using the models directly is prohibitively expensive; therefore, surrogates are constructed to reduce costs. If the optimization is performed using MF surrogates, it will be called MF optimization. Similarly, if the optimization is performed using HF surrogates, it will be called HF optimization. Given a set of input variables, an HF analysis refers to a single computation of the HF model. Similarly, an LF analysis is a single computation of the LF model. The reported cost in time associated with the entire optimization process if MF surrogates are used divided by the

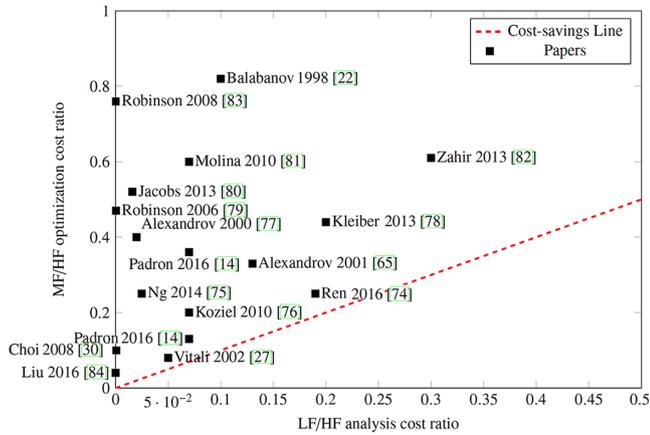


Fig. 2 Cost ratio between a single analysis of the LF surrogate and a single analysis of the HF surrogate vs cost ratio between the optimization process using an MF surrogate and the optimization process using an HF surrogate. The dotted line separates the region where performing the optimization using MF surrogates results in cost savings (upper octant) and the region where there are no cost savings (lower octant).

same cost but using HF models is called *MF/HF optimization cost ratio*. The reported cost in time for a single analysis of the LF divided by the same cost but for the HF is called *LF/HF analysis cost ratio*. In Fig. 2 we present the MF/HF optimization cost ratio as a function of the LF/HF analysis cost ratio. The information presented in Fig. 2 was extracted from 17 papers out of the 102 reviewed that perform optimization in which both the MF/HF optimization cost ratio and the cost and LF/HF analysis cost ratio can be calculated.

One would expect that computational savings would be enhanced when the LF costs are a small fraction of the HF. However, the figure shows that there is no clear relationship between LF/HF analysis cost ratio and MF/HF optimization cost ratio. Because we could not find a clear relationship, we speculate that the relationship between cost and accuracy of the LF model involved might play a big role. That is, very inexpensive models tend to be less accurate and the optimization convergence can be delayed due to this fact. Meanwhile, a more accurate LF model can make the optimizer converge faster, making this a better option even if the LF model is more expensive. Also, having a high correlation between the HF and LF models might lead to better MF surrogate. A high correlation between HF and LF models will usually result in a highly accurate MF surrogate. A high correlation between LF and HF leads to an easy prediction of the discrepancy function between models and therefore a more accurate prediction of the HF model. In addition, the complexity of the resulting model may also influence the cost of the optimization.

To understand the relationship between LF/HF analysis cost ratio and MF/HF optimization cost ratio better, Fig. 3 shows the same data as in Fig. 2 but highlighting field, approach to combine the fidelities, approach to obtain single or MF surrogates coefficients, and type of surrogate used. Overall, there does not seem to be any straightforward relationship between the data.

Figure 3a marks up the different application fields where the optimization was performed. Optimization in fluid mechanics seems to be the most common among the ones that use MF surrogates, but we also have found solid mechanics and electronics. From the figure, it does not appear that the application field determines the usefulness of MF surrogates for optimization.

Figure 3b highlights which of the papers use an optimization approach where the surrogate models are updated in each iteration and which of them are constructed a priori and maintained fixed throughout of the optimization process. The figure does not seem to show any clear trend that suggests more savings to one or another.

Figure 3c distinguishes between deterministic and nondeterministic approaches. Deterministic approaches minimize the difference between the data and the fit. In nondeterministic approaches, the likelihood that the data are consistent with the fit is maximized. There is

no obvious relationship between the gains obtained using deterministic approaches, nondeterministic approaches, or both.

Figure 3d identifies papers by the approach used to combine fidelities. Additive or multiplicative approaches refer to the ones that predict the HF model correcting the LF model response using a discrepancy function or a multiplicative factor, respectively. Comprehensive approaches are the ones that combine additive and multiplicative corrections. Hierarchical models do not explicitly build a surrogate combining LF and HF but use both independently. These models use an algorithm or criterion to decide when to use each fidelity. Space mapping corrects the input variables in space, instead of the output, to predict the HF model. No obvious trends associated with the cases that use the same approach to combine fidelities is observed.

Figure 3e highlights in different colors the surrogates used, showing that there is no clear relationship between the cases that use the same surrogate. Response surface models explore the relationships between independent variables and one or more responses using a design of experiments. These were initially developed to model experimental responses ([75]) and later expanded to numerical responses [76–78]. Kriging ([79] based on Krige's work [80]) is an interpolation method where the data points are interpolated by a Gaussian process model obtained by maximizing the likelihood function of the model for the given data. Co-kriging is the generalization of kriging for multiple sets of data (MF). Support vector regression, developed by Vapnik et al. mainly at AT&T laboratories in the nineties [81,82], allows to introduce error bounds along with the data and it finds a prediction that has an associated error estimation. If interested, the reader can refer to the overview of these surrogate applications in optimization in [1]. Polynomial chaos is a way of representing an arbitrary random variable of interest as a function of another random variable with a given distribution, and of representing that function as a polynomial expansion. It was first introduced by [83] in 1938 and generalized by [84] in 2010. Polynomial chaos expansion is often used in optimization under uncertainty.

Because the literature does not show a clear relationship between LF/HF analysis cost ratio and MF/HF optimization cost ratio, we cannot make a conclusion when to use MF surrogates to save cost. The savings related to MF surrogates, however, can be highly problem dependent. Unless we are dealing with a class of problems of similar structure, the savings that an author reports for one problem could be very different from that for other problems, even if the same methodology is used. This issue is more severe when the savings are not just due to the surrogate construction but for an entire optimization process. For instance, some algorithms can guarantee convergence, meaning that an algorithm will converge to a local critical point of an HF problem regardless of the initial guess. However, the rate of convergence will depend on the relative properties of the LF and HF models.

B. Proposed Guidelines for Reporting on Cost Savings

Time savings while maintaining the desired accuracy is enough of an incentive for applying MF approaches. Unfortunately, we found that it is often difficult to tell from a paper how useful the MF implementation was to accomplish this goal. Among the literature reviewed to build this paper we found one paper, [15], that we consider a good example of an exhaustive savings report. Here, cost, savings, and accuracy were stated. Reporting the cost, savings, and accuracy of the resulting MF method will allow future users to decide whether or not to use MF methods to build approximations of their own problem.

Table 2 presents the savings report extracted from [15] where an airfoil shape was optimized using sequential quadratic programming. Their goal was to minimize the average and standard deviation of the airfoil drag coefficient while maintaining the desired lift coefficient. CFD RANS with Spalart–Allmaras turbulence model was used as the HF model and CFD Euler as the LF model. The RANS HF model had a 23,315 points mesh where 256 were on the airfoil. On the other hand, the Euler LF model had a 6983 points mesh where 128 were on the airfoil. The surrogate used was a stochastic polynomial chaos

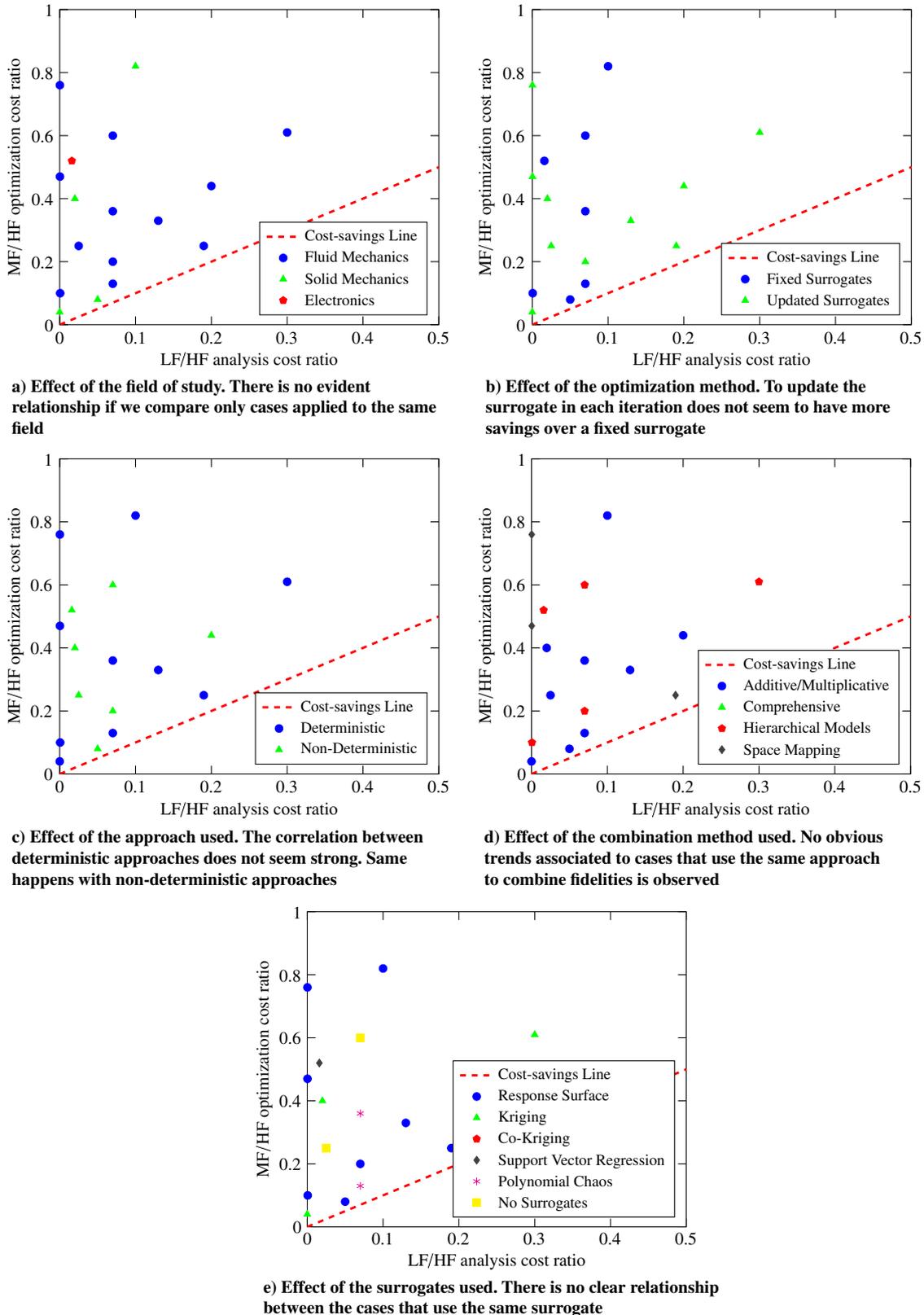


Fig. 3 Same data shown in Fig. 2 but highlighting field, optimization approach, approach to combine the fidelities, approach to obtain single- or multifidelity surrogates coefficients, and type of surrogate used. The dotted line separates the region where performing the optimization using MF surrogates results in cost savings (upper octant) and the region where there are no cost savings (lower octant). Overall, there does not seem to be any straightforward relationship between the data.

expansion and the models were combined through an additive correction. The cost of a single LF analysis is 15 times lower than that of a single HF analysis. The error in the LF model was 18% of the HF model. Two MF surrogates were built: MF0 was built using the information of 1 HF analysis and 17 LF analyses, whereas MF1 was

built with 5 HF and 17 LF analyses. These were compared with an HF build using 17 HF analyses. The cost of the optimization using MF0 was 13% and using MF1 was 36% of the cost of the optimization using the HF surrogate. The objective function was increased (i.e., made poorer) by 5.47% and 0.37% in performance for MF0 and MF1,

Table 2 Optimization cost, savings, and accuracy report given in [15] as a model for authors

Property	Value	Comments
Cost LF/cost HF	0.07	LF = Euler, HF = RANS
Error LF	0.18	HF = 23315 points, LF = 6982 points
Cost MF Opt./cost HF	MF0 = 0.13, Opt. MF1 = 0.36	MF0 = 1HF + 17LF, MF1 = 5HF + 17LF
Objective function increase	MF0 = 5.47%, MF1 = 0.37%	w.r.t. the HF Opt.

It was reported that a single HF analysis costs 15 times the cost of an LF analysis. The LF model error is about 18% compared with the HF model. The optimization time was reduced by 87% with a performance of 95.5% for MF0, and by 64% with a performance of 99.6% for MF1. The overall design was improved by 30%.

respectively, compared with the objective of the HF optimization. Each method ran for 7–10 optimization iterations. The overall airfoil design was improved by 30% for the MF0 and by 33% for the MF1 and HF with respect to the baseline geometry.

In addition, it would be informative to include the accuracy of LF, HF, and MF surrogates obtained at the same computational cost and the cost of the HF and MF surrogates obtained for the same accuracy, if possible. This is done, for example, by [85], where in order to account for accuracy in the calculation of the quantity of interest, a plot is presented giving the root mean square error as a function of the number of samples used. This answers the question of how accurate is the MF method compared with LF and HF models at the same computational cost. In addition, a second plot may report time savings for multiple numbers of samples options. This answers the question of what are the savings associated with the implementation of MF methods compared with the HF surrogate for the same accuracy.

VI. Recommendations on Using MF Surrogates

Between them, the authors have been applying MF surrogates to diverse problems in solid and fluid mechanics for more than 25 years. Even if we cannot make recommendations that apply to all cases we believe that we are able to give some advice about the manner that MF methods should be used that reflect our own experience. Throughout our research, we faced some problems of particular characteristics, which led us to the recommendations summarized below, which the authors would like to give to MF surrogate users.

1) Creating an MF surrogate usually involves substantial investment of time and effort. So it should be undertaken mainly in cases when using an HF surrogate is not an option, because one cannot afford enough samples for an adequately accurate HF surrogate.

2) Adding the scaling parameter ρ that transforms the additive correction to the comprehensive one often results in substantial improvement in accuracy.

3) When the number of HF simulations is severely limited, there is an advantage of using the LF simulations for identifying the most important variables and having the discrepancy function δ include only these variables. The dependence on the other variables may be still adequately captured through the scaled LF function or surrogate (e.g., [67]).

4) When there are multiple candidates for LF simulations, yesterday simulations, that is, simulations that were considered adequate in the past, have been the most promising candidates for our applications.

5) In choosing between candidates for LF simulations, high correlation between LF and HF data is the most important consideration.

6) Selecting an LF simulation that is cheap enough to avoid the need for LF surrogate has two important advantages: a) it often substantially reduces the implementation effort; b) it often avoids a substantial loss of accuracy.

VII. Conclusions

MF surrogates have been a popular topic of research in the past two decades, and substantial progress in accuracy has been achieved. This paper notes that the use of a scaling parameter for the LF data in addition to an additive correction may account for some of this progress. However, based on our survey of a large number of papers, it appears that research is still needed to provide guidelines as to when it is worthwhile to invest the effort in using them. Further research is needed to determine whether applying MF surrogates is worthwhile for a given problem and to select a proper MF surrogate framework for the problem. This effort entails running two or more sets of simulations of different fidelities and selecting surrogates and a method for combining them. There are some indications that the answer may be associated with the bumpiness of the LF function or the bumpiness of the difference between the LF and HF functions. It is also recommended that a quantitative comparison data between LF, HF, and MF models should be reported in future publications. The authors also include some recommendations based on their own experience in the field.

Appendix A: Strategies for Design of Experiment in Multifidelity Surrogates

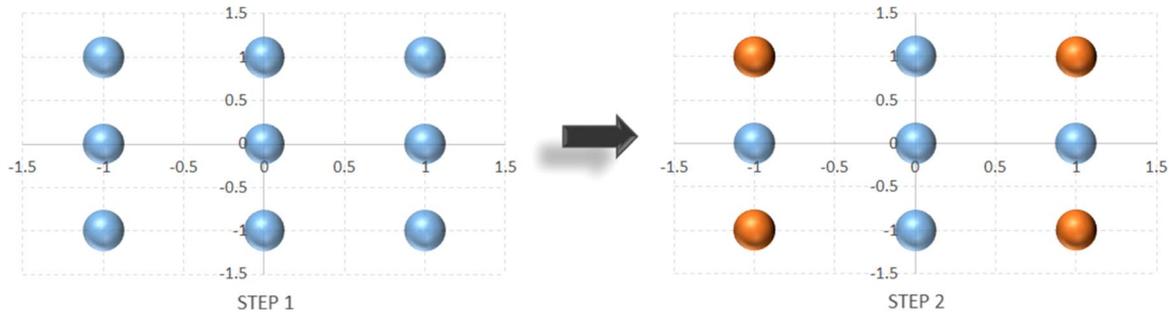
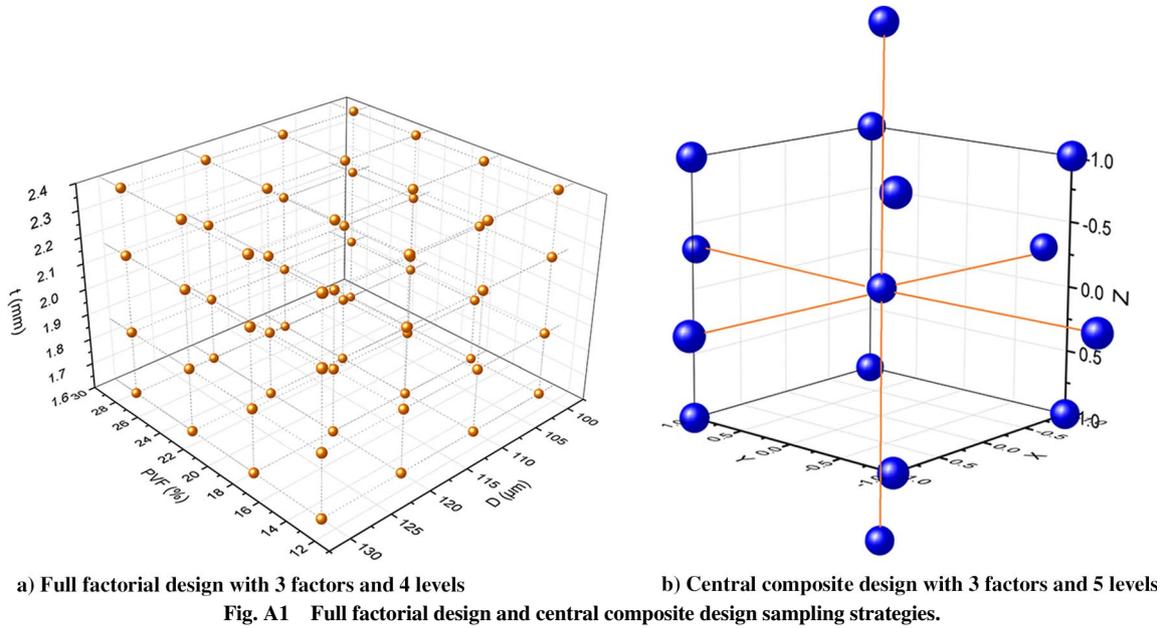
Building surrogates requires a sampling strategy for the generation of a representative group of sample points. Sampling strategies are also related to the accuracy that the surrogate will achieve (see [86]). The simplest sampling methods are grid-based, such as full factorial design, where each variable (factor) is sampled at a fixed number of levels. This method is used for low-dimensional problems (usually less than three variables) (see Fig. A1a). Its application can be seen in [87]. The central composite design method takes the two-level full factorial design and adds to it the minimum number of points needed to provide three levels of each variable so that a quadratic polynomial can be fitted. It is often used when the number of design variables is between three and six (see Fig. A1b). For higher-dimension problems, only a subset of the vertices of the central composite design is used, which is called the small composite design [88]). Full factorial design, central composite design, and small composite design are not flexible in the number of sampling points and domain shape.

Designs of experiments that allow an arbitrary number of samples are usually based on an optimality criterion. For example, in the D-optimal design [89] a subset of a grid in any domain shape is selected by minimizing the determinant of the Fisher information matrix [90]. This reduces the effect of noise on the fitted polynomial, leading to most of the points being at the boundary of the domain. Figure A2 shows the application of D-optimal criterion in a nested sampling design for multifidelity models.

Space-filling methods that spread the points more uniformly in the domain are more popular when the noise in the data is not an issue. When there is substantial noise, the best method is to sample near the domain boundaries using an optimality criterion method. Space-filling methods include Monte Carlo and Latin hypercube sampling. The most common flavor of Latin hypercube sampling attempts to maximize the minimum distance between points, also known as maximin [91] criterion, in order to promote uniformity.

When it comes to MF models, there is the additional issue of the relation between the LF models and HF models sampling points. Nested design sampling strategy generates HF data points as a subset of LF data points or LF points as a superset of HF data points. It was initially developed as a space-filling method for generating additional data sets to complement the existing one using a criterion. For example, Ref. [92] used three optimality criteria: maximin distance criterion, entropy criterion, and centered L_2 discrepancy criterion.

The union of the original sampling points and the additional ones becomes the sampling points for a surrogate built using LF samples, while the additional subset is used for the construction of a surrogate using HF samples [70]. Reference [93] proposes nested design sampling for categorical and mixed factors. Reference [94] compared nested and nonnested design sampling to explore their respective effects on modeling accuracy.

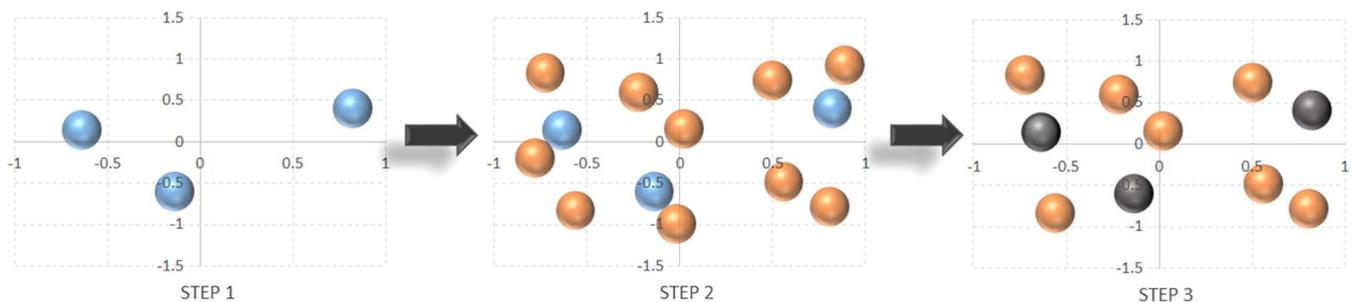


Having the HF data points as a subset of the LF data points makes the parameter estimation easier for methods that build a discrepancy function. A discrepancy function is an additive correction constructed using the relationship between LF and HF data points to estimate the HF response. If they are not a subset, the parameter estimation of the discrepancy function becomes dependent on the parameter determination of the LF surrogate. For instance, co-kriging method models uncertainties using a Gaussian process for both the LF surrogate and the discrepancy function. If the design of experiments satisfies the nested sampling condition, parameters of each Gaussian process model can be estimated separately. Nevertheless, this is not valid for every MF surrogate and, for example, sampling points for Bayesian calibration cannot satisfy the nested condition. However, if we consider only the use of MF surrogate for combining computer

simulation results, we can control the input settings of simulations and therefore satisfy the nested condition.

There are multiple nested designs choices; one possibility is to first generate the design of experiments for the LF model and then select a subset using some criterion. This method is used in [23], where they generated 2107 points in 29-dimensional space using a small composite design for the LF sampling points and then they selected 101 HF sampling points using D-optimality criterion. It is also possible to take the opposite method and generate LF points as a superset of the HF data points.

Reference [95] generated independently the LF and HF sampling points, and then the LF nearest point to each HF point was moved on top of their corresponding *nearest neighbor*, as illustrated in Fig. A3. This method is usually called *nearest*



neighbor sampling. Other MF sampling technique inspired in [95] is the one proposed by [96].

Adaptive sampling methods are strategies used to reduce the number of simulations required to construct a model with a specified accuracy using effective interpolation and sampling methods. These methods are widely applied nowadays, and different ones can be found in the literature. In particular [97] compared two adaptive sampling strategies for generating kriging and radial basis surrogates. They found that both perform better than traditional space filling methods.

It has recently become popular to use LF models and reduced order methods in local searches of parameter space for optimal placement of new design points as we can see in [98,99].

Appendix B: Some Statistics About Multifidelity Model Papers

A large variety of papers that implement MF surrogates were reviewed; we classified them based on six attributes. The attributes are the application, the fidelity type, the method used to construct the MF surrogate, the year published, the paper field, and the surrogate used. Figure B1 gives the reader a sense of how the literature reviewed is distributed throughout the attributes. The six attributes are described as follows:

1) *Application* refers to the kind of problem solved using MF surrogates. We found three main applications: *optimization*, *uncertainty quantification (UQ)*, and *optimization under uncertainty*. *None* refers to the papers that describe a generic procedure without any application.

2) *Types of fidelity* refers to the nature of the fidelity. Discussed further in Sec. B.1.

3) *Method* refers to the criterion used to fit the data in the MF surrogate construction (deterministic method, DM, and non-deterministic method, NDM). *None* refers to papers that use an MF hierarchical method where no MF surrogate is constructed.

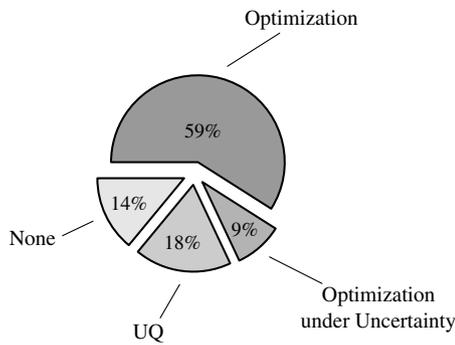
4) *Year published* refers to the year when the paper was released.

5) *Field* refers to the area of the problem solved in the paper. We found that the most common fields are *fluid mechanics* and *solid mechanics*.

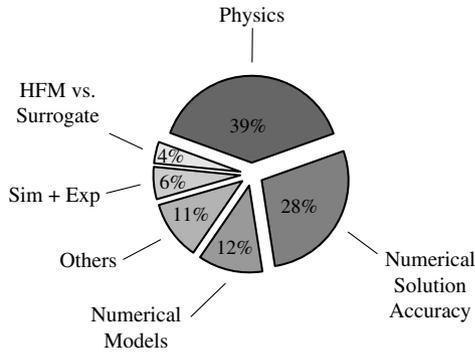
6) *Surrogate* refers to the surrogate used to construct the MF surrogate. *None* represents the papers that use an MF hierarchical method without constructing an MF surrogate.

B.1. Types of fidelity

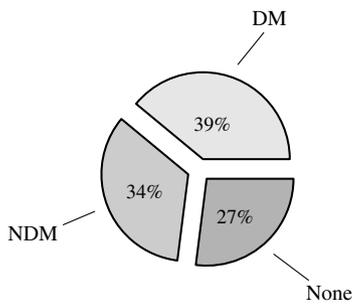
In the literature reviewed, we found that the different types of fidelities are commonly associated with four principal categories:



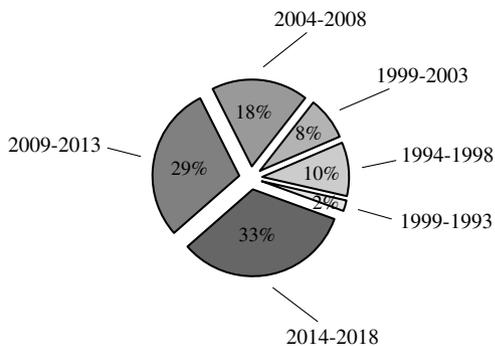
a) Application



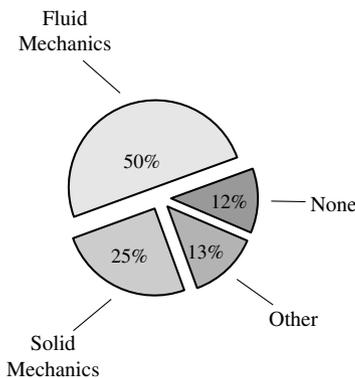
b) Types of fidelity



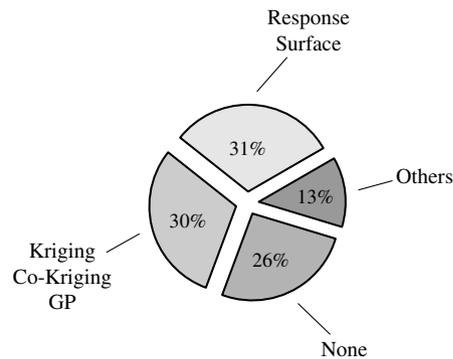
c) Method



d) Year published



e) Field



f) Surrogate

Fig. B1 Proportion of different attributes considered in the MF model papers reviewed; the charts are based on 178 papers.

1) *Physics*: Simplifying the mathematical model of the physical reality, typically changing the differential equations being solved. For example, modeling a flow using Euler inviscid equations corresponds to a lower-fidelity model, and modeling the flow using RANS equations corresponds to a higher-fidelity model and by introducing turbulent effects. Alternatively, the lower fidelity can represent a simplification of the numerical model. Examples include linearization by simplifying the geometry so that the dimensionality of the problem can be reduced, and simplifying the boundary conditions to allow a simpler solution.

2) *Numerical Solution Accuracy*: Changing the discretization model, such as using lower grid discretization or partially converged results as the LF model.

3) *Numerical Models*: Same physical model and assumptions are used but something in the way that the results are computed changes (e.g., 2D RANS simulations as LF model vs 3D RANS simulations as HF model).

4) *Simulation and Experiments*: Using experimental results. In this case, experiments are considered the highest fidelity.

In fluid mechanics the main models found were *analytical expressions, empirical relations, linear approximations, potential flow, Euler, RANS, and direct numerical simulations*. Table B1 shows papers that use these models as LF models and HF models.

Table B2 includes extra categories found in fluid mechanics: *dimensionality* (e.g., 2D/3D), *coarse vs refined* analysis, *simulations vs experiments, transient vs steady*, and *semiconverged vs converged* solutions.

Other models that are not included in Table B1 or Table B2 are:

1) Simplifying physics found in [152], where an earth penetrator problem is simplified by assuming a rigid penetrator.

2) In [153], where the physics are simplified by assuming constant instead of variable material properties.

3) In [147] where the LF model is a RANS simulation with simplified geometry and the HF model is a RANS simulation with full geometry.

4) In [154], where the fidelity distinction is based on the number of Monte Carlo samples to be combined.

In solid mechanics the main models found were analytical expressions, empirical relations, numerical linear approximations, numerical nonlinear approximations, and coarse vs refined analysis.

Table B3 shows papers that use these models as LF models and HF models. Other models not included in Table B3 are found in [155], where LF models and HF models are *isothermal* and *nonisothermal* analysis, respectively.

Table B4 includes additional models found in solid mechanics, including *dimensionality* (e.g., 2D/3D), *coarse vs refined, simulations vs experiments*, and *boundary condition simplification* (e.g., infinite plate vs finite plate).

Table B1 Fluid mechanics-oriented papers per LF model and HF model used

Reference	Fidelity type						
	An	Em	Li	PF	Eu	RANS	DNS
[100,101]	LF/HF	---	---	---	---	---	---
[29,35]	LF	---	HF	---	---	---	---
[1,10,102–105]	---	LF	HF	---	---	---	---
[7,106–108]	---	LF	---	---	---	HF	---
[21,27,41,109–114]	---	---	LF	---	HF	---	---
[94,115–118]	---	---	LF	---	---	HF	---
[4,16,119,120]	---	---	---	LF	---	HF	---
[15,46,121–125]	---	---	---	---	LF	HF	---
[5,126]	---	LF	---	---	---	---	HF

An, analytical; DNS, direct numerical simulations; Em, empirical; Eu, Euler; Li, linear; PF, potential flow; RANS, Reynolds-averaged Navier–Stokes.

Table B2 Fluid mechanics-oriented papers by LF model and HF model used

Fidelity type	Reference
Dimensionality	[10] 2D/3D Eu, [127] 1D/3D RANS+TM, [4] 2D/3D URANS, [128] 2D/3D, [14] 1D/2D RANS, [129] 1D/2D Li, [130] 1D/3D RANS, [131] 1D/3D RANS, [6] 1D,2D/3D RANS
Coarse/refined	[66] Eu, [132] RANS, [133] Eu, [115] Eu, [31] Li/Eu, [134] Li, [8] RANS, [135] MFF, [136] MHD, [137] Eu, [17], Eu[138] Eu, [139] Eu, [140] RANS, [141] OB, [142] RANS, [143] RANS, [144] RANS, [145] Eu/RANS, [146] RSM
Exp./Sim.	[47] Euler/MHD, [147] PF/Em, [148] RANS, [149] RANS
Semiconverged/converged	[8] RANS, [17] Eu, [150] Eu
Steady/transient	[61] AE, [151] Eu, [12] RANS, [144] TM

The categories are dimensionality (e.g., 2D/3D), coarse vs refined analysis, simulations vs experiments, transient vs steady, and semiconverged vs converged solutions. The physical model used by each paper was also assigned where AE, aeroelastic equations; Em, empirical; Eu, Euler; Li, linear; MFF, multiphase flow; MHD, magnetohydrodynamics; OB, Oberbeck–Boussinesq equations; PF, potential flow; RANS, Reynolds-averaged Navier–Stokes; RSM, Reynolds stress model; TM, thermomechanical equations; TM, turbulence method; URANS, unsteady RANS.

Table B3 Solid mechanics-oriented papers per type of analysis used to determine fidelity

Reference	Fidelity type			
	An	Em	Li	NL
[32]	LF	---	HF	---
[22,30]	---	LF	HF	---
[22]	---	LF	---	HF
[114,156–162]	---	---	LF	HF

An, analytical; Em, empirical; Li, linear; NL: nonlinear.

Table B4 Solid mechanics-oriented papers per type of fidelity used besides analysis type

Fidelity type	Reference
Dimensionality	[163] 1D/2D Li, [164] 1D/3D, [165] 2D/3D, [25] 2D/3D Li, [33] 2D/3D Li, [166] 2D/3D NL
Coarse/refined	[23] Li, [9] NL, [167] Li, [168] NL, [20] Li, [44] Li, [169] Li, [34] NL, [62] NL, [170] Li, [59] Li, [60] Li
Exp./Sim.	[171] Li
Boundary conditions	[26] Li, [172] Li

The categories are dimensionality (e.g., 2D/3D), coarse vs refined and boundary condition simplification (e.g., infinite plate vs finite plate). The model used by each paper was also assigned, where Li, linear; NL, nonlinear.

We also reviewed some papers whose field was not fluid or solid mechanics; these papers are listed below:

1) In electronics the most common method is *coarse vs refined analysis* [173–175], although [42] used *steady vs transient* models. Reference [176] used as HF an electromagnetic simulation model, while the LF is an analytical expression.

2) In robotics, in [177], the fidelities corresponded to complexity determined by resources available to the robot.

3) Some of the papers test their methods using mathematical functions, and there is not an application to a particular field. For example, *analytical function vs analytical approximations of the function* are shown in [3,45,95,98,99,178–180].

4) In the category of methods for uncertainty analyses with no application to a field in particular, we found [40,85,181–183]. In [15,182] the types of fidelity were less and more accurate uncertainty analysis. In [85] LF models were used to aid in the construction of the biasing distribution for importance sampling, and a small number of HF samples are used to get an unbiased estimate. Reference [183] employed an iterative method that used LF surrogates for approximating coupling variables and adaptive sampling of the HF system to refine the surrogates in order to maintain a similar level of accuracy as uncertainty propagation using the coupled HF multidisciplinary system.

Acknowledgments

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