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APPLICATION OF SOFT COMPUTING

Recent advances and applications of surrogate models for finite element method computations: a review

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Abstract

The utilization of surrogate models to approximate complex systems has recently gained increased popularity. Because of their capability to deal with black-box problems and lower computational requirements, surrogates were successfully utilized by researchers in various engineering and scientific fields. An efficient use of surrogates can bring considerable savings in computational resources and time. Since literature on surrogate modelling encompasses a large variety of approaches, the appropriate choice of a surrogate remains a challenging task. This review discusses significant publications where surrogate modelling for finite element method-based computations was utilized. We familiarize the reader with the subject, explain the function of surrogate modelling, sampling and model validation procedures, and give a description of the different surrogate types. We then discuss main categories where surrogate models are used: prediction, sensitivity analysis, uncertainty quantification, and surrogate-assisted optimization, and give detailed account of recent advances and applications. We review the most widely used and recently developed software tools that are used to apply the discussed techniques with ease. Based on a literature review of 180 papers related to surrogate modelling, we discuss major research trends, gaps, and practical recommendations. As the utilization of surrogate models grows in popularity, this review can function as a guide that makes surrogate modelling more accessible.

Keywords Surrogate model · Surrogate-assisted optimization · Sensitivity analysis · Uncertainty quantification · Finite element method

1 Introduction

The methods of numerical analysis, such as the finite-element method (FEM), computational fluid dynamics (CFD), or structural finite-element analysis (FEA), are routinely employed to perform analysis of complex systems and structures where obtaining an analytical solution may be either difficult or impossible. Such analyses are becoming ubiquitous in evaluating and optimizing design, reliability, and maintenance of complex systems and structures in a broad range of various industrial applications including aerospace (Yan et al. 2020), automotive (Berthelson et al. 2021), architecture (Westermann and Evins 2019), biomedical engineering (Putra et al. 2018), chemical engineering (Bhosekar and Ierapetritou 2018), and many others.

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However, these computer simulations tend to be very computationally demanding because of their intrinsically detailed description of the studied systems. These engineering problems based on computer models also require the computation of thousands of simulations in order to construct a suitable solution, requiring a large computational budget (Alizadeh et al. 2020). Additionally, because of their high fidelity, various issues in performing computer simulations can occur regardless of how much computer power can be used. Even the recent advance of parallel and pooling (Kudela and Popela 2020) computing methods, that carry out many calculations or executions of processes simultaneously, do not seem to be very helpful (Grama et al. 2003).

The principle purpose of using surrogate models (or metamodels) is to approximately emulate the expensive-to-evaluate high-fidelity models, such as a FEM-based model, employing computationally less costly statistical models. These surrogates are constructed based on a relatively low number of simulation input and output data, that are computed employing the high-fidelity expensive computations.

After the surrogate is validated to achieve a sufficient level of approximation of the FEM-based model, its utilization to predict the outputs of the high-fidelity model can be done almost instantly.

There are several features of a given problem, including its linearity/nonlinearity, the required accuracy level, the size (input dimensions) of the problem, the required amount of information, the speed of the computations, the number of samples, and the availability of convenient software tool that impact the appropriateness of a given surrogate (Alizadeh et al. 2020). It is possible to divide the use of surrogate models into three classes of problems. The first class contains the most fundamental utilization of surrogates—building and validating surrogate models and using them for prediction. The second class of problems deal with sensitivity analysis of the resulting models and different ways of quantifying the impact of uncertain parameters, that may influence the behaviour of the modelled systems. The third class is commonly called surrogate-assisted optimization, in which the objective function used for optimization is prohibitively expensive to compute and the information about its derivative is not available.

The primary motivation of this paper lies in investigating recent advances and applications of surrogate models for FEM-based computations. Although the utilization of surrogate models is growing in popularity, a text summarizing the state-of-the-art and recent developments (especially for FEM-based computations) was missing. The novelty of this paper is in encapsulating the state-of-the-art in surrogate modelling for FEM-based computations from both the theoretical and application perspectives. We also expect this work to function as a guide in the selection of the suitable approximation models for applications of computationally expensive high-fidelity FEM-based problems. This review emphasizes the differences between employing surrogates for the three above mentioned problem classes and gives a comprehensive overview of surrogate modelling and corresponding techniques. The main contributions of this paper, obtained by assessing 180 papers related to surrogate modelling, are the following:

- Analysis of the state-of-the-art in surrogate modelling techniques.
- Review of the recent advances in using surrogate models for FEM computations—highlighting both theoretical and application developments in model building and validation, sensitivity analysis and uncertainty quantification, and surrogate-assisted optimization.
- Description of available software tools.
- Identification of trends and research gaps.

The rest of the paper is organized as follows. Section 2 discusses the basics of surrogate modelling: sampling, model validation methods, and various model choices for surrogates and the underlying mathematical formulas. Section 3 describes the sensitivity analysis and uncertainty quantification approaches and their applications in FEM-based computations. In Sect. 4, we give a thorough overview of recent methodological advances and applications of surrogate-assisted optimization. Section 5 lists the most widely used as well as recently developed software tools. Section 6 summarizes the trends, research gaps, and recommendations extracted from the considered literature. Finally, conclusions and suggestions for further research are drawn in Sect. 7.

2 Surrogate modelling

First, we discuss the most frequently utilized approaches for building and validating the surrogates of the expensive-to-compute functions. We will deal with a surrogate $\hat{f}(x)$ of the function $f : R^d \rightarrow R$, where $x = (x_1, x_2, \ldots, x_d)$ is the input vector, d is the number of dimensions of the problem, and we have a single output y. The upper and lower bounds on the input (or design) vector are known and are denoted as $x_L \leq x \leq x_U$.

2.1 Sampling and model validation

After determining the input parameters (or the design space) of the model, we must select the data points (or designs) to evaluate for building the surrogate model. This process is usually called sampling, and sometimes is also referred to as design of experiments (DOE). The number of samples we choose to evaluate and their quality has a direct impact on the precision of the surrogate. As evaluating the data points comprises of the computation of the true function (in this case, running the expensive simulation), sampling is the source of significant computational costs. Maintaining the quality of the surrogate model without suffering prohibitive sampling cost can be achieved by using appropriate sampling strategies (Bhosekar and Ierapetritou 2018).

Sampling strategies can be divided into stationary sampling and adaptive sampling. The methods of stationary sampling are based upon geometry or patterns (such as full/half factorial design, or grid sampling) and approaches based on the DOE literature (orthogonal sampling, Box–Behnken design, etc.). Among the most frequently used used strategies of stationary sampling are the Latin Hypercube Sampling (LHS) (McKay et al. 1979), the maximin sampling (Johnson et al. 1990), and the sampling techniques of Morris and Mitchell (1995).

Conversely, adaptive sampling starts from fewer samples which are usually computed by using one of the stationary sampling strategies, but new sample points are determined sequentially. The goal of adaptive strategies is to decrease sampling requirements by evaluating samples that are expected to increase the precision of the resulting surrogate. Most adaptive sampling approaches use various criteria for balancing the trade-offs between exploring the under-explored regions of the design space (exploration) and refining the regions close to the already evaluated samples for improved performance (exploitation). A frequent use of such an approach is within surrogate-assisted optimization in which exploration is applied to deal with local optima while exploitation aims at improving on the best design found so far. In the case of Kriging surrogates, one of the popular approaches is based on the Expected Improvement (EI) criterion (Jones et al. 1998), while for Radial Basis Function (RBF) surrogates, an analogous quantitative measure is achieved using a so called bumpiness criterion (Gutmann 2001).

In general, the approaches that address this exploration /exploitation trade-off have been demonstrated to attain better surrogate accuracy with a lower number of samples (Provost et al. 1999). The approaches based on a space-filling sequential design were also studied in Crombecq et al. (2011). Here, the authors developed a group of sequential sampling approaches which exhibit performance competitive with one-shot or stationary experimental designs. It is possible to reformulate the adaptive sampling problem as an optimization problem (Cozad et al. 2014), where the objective function measures the discrepancy between the expensive-to-compute function $f(x)$ and its surrogate $\hat{f}(x)$

$$\max\left(\frac{f(x)-\hat{f}(x)}{f(x)}\right)^2, \quad x_L \leq x \leq x_U.$$

Other contemporary methods make use of ranking the exploitation and the exploration and weighing them as needed. Garud et al. (2017) developed such a method, where a metric that consisted of two different measures for exploitation and exploration was employed. As the exploitation metric, they quantified the impact of the new sample point added near a point that was already sampled by the so called departure function. As the exploration metric, they used the sum of squares of the distances between the new sample and all the previously evaluated samples. By estimating the prediction variance of a surrogate model by the jackknifing technique, (Eason and Cremaschi 2014) suggest a different adaptive sampling method where the surrogate model is constructed using ANN and sample points that exhibit high prediction variance are selected. Such a method of adaptive sampling has the advantage of not being specific to the selection of particular surrogate models.

Evaluating the reliability of the constructed surrogate model constitutes one of the most important concerns—relying on a flawed surrogate model can result in a misuse of computational resources, and produce negative effects on prediction, optimization, or the resulting analyses. Validation of surrogate models is the procedure of evaluating the performance of the resulting surrogate models where, apart from measuring their accuracy, validation techniques are frequently utilized in the selection of a suitable surrogate model from a collection of candidate models and in tuning of its hyperparameters.

A common approach is to employ resampling techniques, such as bootstrapping or cross-validation (Forrester and Keane 2009). In the cross-validation approaches, the training data for a surrogate model are randomly partitioned into q subsets of roughly equal size. These subsets are then in turn removed from the set of the training data while the fitting of the model is performed on data that remain. Afterwards, the subset that was removed is predicted by the model that was fitted to the data that remained. Once every subset has been removed, the calculations of n predictions denoted by $\hat{y} = (\hat{y}^{(1)}, \hat{y}^{(2)}, \ldots, \hat{y}^{(n)})$ of the n observed data points $y = (y^{(1)}, y^{(2)}, \ldots, y^{(n)})$ will be performed. The difference between the observations and the obtained predictions, i.e., the prediction error, is quantified by using various validation metrics. One of the most frequently used metrics for validation is the Mean Squared Error (MSE), calculated as

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \hat{y}^{(i)})^2.$$

Using $q = n$, one can obtain an error estimate that is almost unbiased, but its variance is often very large. Hastie et al. (2001) suggested using a bit larger subsets, that have $q = 5$ or 10.

A similar method, but one which allows repeated samples in the training data is bootstrapping. By enabling the repetition of the samples in the set that is designated for building the model, we obtain a training set that has the same size as the actual data. Generally, for bootstrapping the number chosen of subsets q is larger than in the case of cross-validation. Apart from the already mentioned MSE, there are other commonly used validation metrics such as the explained variance score, the mean absolute error, the median absolute error, and the R^2 score. These metrics, along with the corresponding mathematical formulations, can be found in Table 1, where $\bar{y}$ denotes the mean predicted value. More details on various resampling approaches that are used for validation of surrogate models are discussed by Bischl et al. (2012).

Table 1 Conventionally used metrics for surrogate validation (Hastie et al. 2001)

Validation metric	Mathematical formula
R^2 score	$1 - \frac{\sum_{i=1}^{n}(y^{(i)}-\hat{y}^{(i)})^2}{\sum_{i=1}^{n}(y^{(i)}-\bar{y})^2}$
Mean absolute error	$\frac{1}{n}\sum_{i=1}^{n} \mid y^{(i)} - \hat{y}^{(i)} \mid$
Median absolute error	$\mathrm{median}(\mid y^{(1)} - \hat{y}^{(1)} \mid, \ldots, \mid y^{(n)} - \hat{y}^{(n)} \mid)$
Explained variance score	$1 - \frac{\mathrm{Var}(y-\hat{y})}{\mathrm{Var}(y)}$

2.2 Model choice

2.2.1 Response surfaces and linear regression

The classic polynomial response surface model (RSM) (Box and Draper 1987) is the original and to this day one of the most frequently employed types of surrogate models in engineering design (Forrester and Keane 2009). In the RSM method, the surrogate is represented as a linear combination of polynomial functions (mostly linear and quadratic) of the input variables. A so called first-order RSM has the following form:

$$\hat{f}(x, a) = a_0 + a_1 x_1 + \cdots + a_m x_m$$

where the vector $a = (a_0, \ldots, a_m)^T$ is obtained by minimizing the sum of squared errors between the value from the expensive-to-compute function and the value predicted by the surrogate model. This (least squares) minimization problem is unconstrained and can be written as

$$\min \mid\mid Xa - y \mid\mid_2^2,$$

where the matrix X of size n by $m + 1$ has all elements in its first column equal to 1 while the remaining columns contain the input vector. In the case of ordinary least squares, there is an analytical solution in the form $a = (X^T X)^{-1} X^T y$. If one or more of the input vector components x_i are perfectly correlated, the resulting matrix $X^T X$ can become singular (or can be very badly conditioned), which results in the coefficients a not being uniquely defined. Such an issue is usually approached by decreasing the number of input variables by prescreening, or by using regularization methods, such as ridge regression or lasso (Hastie et al. 2001).

Higher order polynomials are also commonly used, especially if there is a curvature in the problem. For example, a second-order model has the following form:

$$\hat{f}(x, a, \alpha) = a_0 + \sum_{i=1}^{m} a_i x_i + \sum_{i=1}^{m} \alpha_{ii} x_i^2 + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \alpha_{ij} x_i x_j,$$

where the coefficients of a and α are again obtained by solving a least squares problem. Polynomial surrogates remain generally not well suited for the nonlinear, multi-dimensional, multi-modal design landscapes one deals with in engineering unless the ranges of the considered variables are made sufficiently small, e.g. in trust-region methods (Forrester and Keane 2009).

Also, in problems that are high-dimensional it may be impossible to sample enough data required for the estimation and construction of all except the low order polynomials. On the other hand, for problems that are not high-dimensional, display low modality (or unimodality), or where data are relatively inexpensive to compute, the use of polynomial surrogates may be an attractive (and correct) choice. Moreover, the individual terms of the polynomial expression computed by the methods mentioned above can give insight about the problem itself, e.g. the role of the individual inputs is quite easily judged by the value of the corresponding coefficient.

2.2.2 Kriging

Kriging refers to a surrogate model that is based on Gaussian process modelling (and is sometimes called Gaussian process regression Rasmussen and Williams 2006). The method first originated in geostatistics in a paper by Krige (1951) and became popular after its use for analysis and of various computer experiments (Sacks et al. 1989). Nowadays, it is among the most widely used methods for building surrogate models.

A Kriging surrogate model can be formulated as follows:

$$\hat{f}(x) = \sum_{i=1}^{m} a_j g_j(x) + \varepsilon(x), \tag{1}$$

where $g_j(x)$ denotes the m independent (and known) basis functions which describe the trend of prediction of the mean at the point x, a_j denotes the unknown parameters, and $\varepsilon(x)$ denotes the random error at the point x which follows a normal distribution with a zero mean. The Kriging predictor can be then formulated in the following way

$$\hat{f}(x) = g(x)^T a^* + r(x)^T \alpha^*,$$

where $g(x) = [g_1(x), \ldots, g_m(x)]^T$, a^* denotes the vector of the generalized least-square estimates of $a = [a_1, \ldots, a_m]^T$, $r(x)$ denotes the correlation vector of size $n \times 1$ between $\varepsilon(x)$ and $\varepsilon(x_i)$, and a^* and α^* are computed as

$$a^* = (G^T R^{-1} G)^{-1} G^T R^{-1} y,$$
$$\alpha^* = R^{-1}(y - Ga^*),$$

where R denotes the $n \times n$ covariance matrix whose (i, j) element describes the correlation between $\varepsilon(x^{(i)})$ and $\varepsilon(x^{(j)})$,

$G = [g(x^{(1)}), \ldots, g(x^{(n)})]^T$ is $n \times m$ matrix, and y denotes the observations at the available points. The variance of the process, denoted by σ^2, can be computed as

$$\sigma^2 = \frac{1}{n}(y - G^T a^*)^T R^{-1}(y - G^T a^*).$$

In the Kriging surrogate model, we assume that the random variables $\varepsilon(x)$ are correlated in accordance to the correlation model $R(\cdot, \cdot)$, which is parameterized by a collection of hyperparameters θ. These hyperparameters are usually computed by using maximum likelihood estimation (MLE) methods. One can find a comprehensive treatment of MLE in the context of Kriging in Kaymaz (2005).

Depending on the particular selection of the model for mean prediction $g(x)^T a$ in (1), there exist different modifications of Kriging: universal Kriging (also called Kriging with trend), ordinary Kriging, and simple Kriging. In simple Kriging we assume that the term $g(x)^T a$ is a known constant while in ordinary Kriging we assume it is an unknown constant. In universal Kriging we assume that $g(x)$ is any other (prespecified) function of x. Frequently, $g(x)$ has the form of a polynomial regression (of a lower order). Conventionally, the selection of the order of the polynomial is done empirically. On the other hand, this kind of a non-adaptive framework can make the modelling rather ineffective. To bypass this issue, blind Kriging (Joseph et al. 2008; Hung 2011) and similar methods (Kamiński 2015) are used.

Another important feature of Kriging is the selection of a suitable covariance function (Lirio et al. 2014). Usually, the covariance functions employed with Kriging surrogates are stationary ones which can be formulated as

$$R(x, x') = \prod_j \psi_j(\theta, m_j), \quad m_j = x_j - x'_j.$$

A correlation function expressed in this way enjoys two attractive properties. The first one is that it is possible to express the correlation function for multivariate functions by a product of several one-dimensional correlations. The second one is that the correlation is stationary, depending only on the distance m_j between the two points x and x'.

Frequently employed correlation models can be found in Table 2, where Γ is the Gamma function, K_{v_j} the modified Bessel function of order v_j, and the parameter $v_j > 0$ controls the differentiability of the Matern correlation model. Chen et al. (2016) compared several of the mentioned correlation models, showing a worse performance of the squared exponential correlation model in comparison to the exponential correlation one. On the other hand, an important note is that the generalized exponential correlation model needs twice as many hyper-parameters ($2d$) when compared to squared exponential correlation one. The authors also suggested using the Matern model (see Table 2) as a better alternative to the exponential correlation one.

2.2.3 Radial basis functions

RBFs (Broomhead and Lowe 1988) compute a weighted sum of prespecified simple functions to approximate complex design landscape. Sobester (2003) used an analogy of mimicking the characteristic timbre of a musical instrument by a synthesizer that uses a weighted combination of different tones. Given n different sample points, the RBF surrogates are written as

$$\hat{f}(x) = \sum_{i=1}^{n} w_i \psi(|| x - x^{(i)} ||_2),$$

where w_i denotes the weight which is computed using the method of least-squares, and ψ is the chosen basis function. There are several (symmetric) radial functions that can serve as a basis function, with the most widely ones summarized in Table 3.

An important note is that unlike response surface methods, RBF does not belong to the regression techniques. Conversely, RBF is broadly considered to be an interpolation method. This means that RBFs, in contrast with regression techniques, give exact result at the points that were already sampled. There is still no firm conclusion in the literature that would decisively show whether some of the mentioned basis functions are better than the others.

2.2.4 Support vector regression

SVR is based on the theory of support vector machines (SVM), that originated at AT&T Bell Laboratories (Vapnik 1995). In our context of surrogate-assisted engineering design, it is arguably more fitting to view SVR as the extension of the RBF techniques rather than of the SVMs (Forrester and Keane 2009).

One of the main attributes of the SVR methods is that they give us the possibility to prescribe a margin (δ) within which one can accept errors present in the sampled data without having negative effect on the prediction capabilities of the resulting surrogate models. This might be helpful in situations when the sample data contain random errors because of, for instance, a finite size of the mesh, because by performing an analysis of mesh sensitivity we can determine an appropriate value of δ.

The basic shape of an SVR prediction has the familiar form of a weighted sum of prescribed basis functions ψ, which have weights w, and are added to the "base" term μ. These are calculated in a different way to their Kriging and RBF counterparts, yet they contribute to the surrogate prediction in the exact same manner:

Table 2 Frequently employed correlation models for Kriging surrogates (Kleijnen 2017)

Name	Correlation model
Exponential	$\psi_j(\theta, m_j) = \exp(-\theta_j \mid m_j \mid)$
Generalized exponential	$\psi_j(\theta, m_j) = \exp(-\theta_j \mid m_j \mid^{\theta_{n+1}}), \quad 0 \le \theta_{n+1} \le 2$
Gaussian	$\psi_j(\theta, m_j) = \exp(-\theta_j m_j^2)$
Linear	$\psi_j(\theta, m_j) = \max\{0, 1 - \theta_j \mid m_j \mid\}$
Spherical	$\psi_j(\theta, m_j) = 1 - 1.5\xi_j + 0.5\xi_j^2, \quad \xi_j = \min\{1, \theta_j \mid m_j \mid\}$
Cubic	$\psi_j(\theta, m_j) = 1 - 3\xi_j^2 + 2\xi_j^3, \quad \xi_j = \min\{1, \theta_j \mid m_j \mid\}$
Spline	$\psi_j(\theta, m_j) = \begin{cases} 1 - 5\xi_j^2 + 30\xi_j^3, & 0 \le \xi < j \le 0.2 \\ 1.25(1-\xi_j^3), & 0.2 < \xi_j \le 1 \\ 0, & \xi_j > 1 \end{cases}, \xi_j = \theta_j \mid m_j \mid$
Matern	$\psi_j(\theta, m_j) = \frac{1}{\Gamma(v_j)2^{(v_j-1)}}(\theta_j \lvert m_j \rvert)^{v_j} K_{v_j}(\theta_j \mid m_j \mid)$

Table 3 Commonly used radial basis functions (Bhosekar and Ierapetritou 2018)

Name	Radial basis function
Linear	$\psi(r) = r$
Cubic	$\psi(r) = r^3$
Multi-quadric	$\psi(r) = \sqrt{r^2 + \gamma^2}, \ \gamma > 0$
Inverse multi-quadric	$\psi(r) = \frac{1}{\sqrt{r^2+\gamma^2}}, \ \gamma > 0$
Thin plate spline	$\psi(r) = r^2 \ln(r)$
Gaussian	$\psi(r) = \exp(-\frac{r^2}{\gamma}), \ \gamma > 0$

$$\hat{f}(x) = \mu + \sum_{i=1}^{n} w_i \psi(x, x^{(i)}).$$

For a linear mapping, this can be rewritten using an inner product $\langle \cdot, \cdot \rangle$ as

$$\hat{f}(x) = \mu + \langle w, x \rangle. \tag{2}$$

Finding the weights that minimize the margin δ corresponds to solving the following convex optimization problem

$$\begin{aligned} \min \ & \frac{1}{2} \mid\mid w \mid\mid_2^2 \\ \text{subject to} \ & y^{(i)} - \langle w, x^{(i)} \rangle - \mu \le \delta, \quad i = 1, \ldots, n, \\ & \langle w, x^{(i)} \rangle + \mu - y^{(i)} \le \delta, \quad i = 1, \ldots, n. \end{aligned}$$

As there might not be a feasible solution to the optimization problem above, an extension using slack variables ξ^+ and ξ^- is used in practice

$$\begin{aligned} \min \ & \frac{1}{2} \mid\mid w \mid\mid_2^2 + \gamma \sum_{i=1}^{n} (\xi_i^+ + \xi_i^-) \\ \text{subject to} \ & y^{(i)} - \langle w, x^{(i)} \rangle - \mu \le \delta + \xi_i^+, \quad i = 1, \ldots, n, \\ & \langle w, x^{(i)} \rangle + \mu - y^{(i)} \le \delta + \xi_i^-, \quad i = 1, \ldots, n, \\ & \xi_i^+, \xi_i^- \ge 0, \quad i = 1, \ldots, n, \end{aligned}$$

where γ is a regularization parameter that controls the desired trade-offs between the complexity of the model and a level for which errors larger than δ are allowed. Using Lagrangian duality theory, a dual optimization model can be constructed

$$\begin{aligned} \max \ & -\frac{1}{2} \sum_{i,j=1}^{n} (\alpha_i^+ - \alpha_i^-)(\alpha_j^+ - \alpha_j^-) \langle x^{(i)}, x^{(j)} \rangle \\ & - \delta \sum_{i=1}^{n} (\alpha_i^+ + \alpha_i^-) + \sum_{i=1}^{n} y^{(i)} (\alpha_i^+ - \alpha_i^-) \qquad (3) \\ \text{subject to} \ & \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) = 0 \\ & \alpha_i^+, \alpha_i^- \in [0, \gamma], \quad i = 1, \ldots, n, \end{aligned}$$

where the resulting weights are computed as

$$w = \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) x^{(i)},$$

and, to compute μ the Karush–Kuhn–Tucker (KKT) conditions have to be used. Substituting into (2), we get

$$\hat{f}(x) = \mu + \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) \langle x^{(i)}, x \rangle.$$

The advantage of the Lagrangian formulation is that we can extend the above mentioned model beyond the usual linear regression to different basis functions (which are known in the support vector literature as kernels), that are able to approximate more complex landscapes, by the so-called kernel trick. The procedure amounts to replacing the inner product $\langle \cdot, \cdot \rangle$ with a kernel function ψ, which needs to satisfy the conditions for a Mercer kernel. The most popular choices

Table 4 Commonly used kernel functions (Hastie et al. 2001)

Name	Mercer kernel function
Gaussian	$\psi(x^{(i)}, x^{(j)}) = \exp(-\frac{\|\|x^{(i)}-x^{(j)}\|\|^2}{\sigma^2}),\ \sigma > 0$
Linear	$\psi(x^(i), x^(j)) = \langle x^{(i)}, x^{(j)}\rangle$
d degree homogeneous polynomial	$\psi(x^{(i)}, x^{(j)}) = (\langle x^{(i)}, x^{(j)}\rangle)^d$
d degree inhomogeneous polynomial	$\psi(x^{(i)}, x^{(j)}) = (\langle x^{(i)}, x^{(j)}\rangle + c)^d$

for ψ are shown in Table 4. Whichever form of the kernel function is selected, the method for computing support vectors stays the same—as the properties of the Mercer kernel guarantee the optimization problem (3) is a convex quadratic one it can be readily solved by employing quadratic programming solvers.

2.2.5 Artificial neural networks

Artificial neural networks (ANNs) form a group of surrogate models that take inspiration from the biological functions found in the brain and in the nervous system. The structure of an ANN is usually represented by a system of mutually interconnected "neurons". These neurons in an ANN contain various primitive functions, and the connections between the neurons have numeric weights that are computed according to the input data. There are three elements that guide the construction of an ANN: a network topology (single or multiple layers), primitive functions related to the neurons, and a learning algorithm used to compute the corresponding weights. Most widely used paradigm of an ANN consists of a so-called multilayer perceptron (MLP) that is based on feed-forward (supervised) learning, and on the back-propagation algorithm (Sun and Wang 2019).

Among the various ANNs architectures, multilayer feed-forward neural network (MFFNN) are among the most frequently used ones (Chatterjee et al. 2019). In the MFFNN the neurons are organized into three layers: the input layer, the hidden layer, and the output layer. Note that the number of layers in MFFNN can be larger than just one and usually a convergence study is needed to find the right number of hidden layers. Similarly, the number of neurons in the hidden layers needs to be chosen based on a suitable convergence criterion.

The learning capabilities of an MLP architecture can be improved by using more hidden layers, and/or neurons in the hidden layers. On the other hand, there are trade-offs between the learning/prediction capabilities the network and its size. To address these issues, the approaches of "deep learning" have recently gained increased attention, although deep learning is only a subconcept under the ANNs. When compared to its conventional MLP counterparts, the deep learning approaches utilize more training layers and characterized layers (e.g. pooling and convolutional layers).

2.2.6 Polynomial chaos expansion

The polynomial chaos expansion (PCE) is a method for producing responses of stochastic systems which was developed by Wiener (1938). Afterwards, generalized results were introduced by Xiu and Karniadakis (2002) for different discrete and continuous system from the so-called Askey scheme.

Let $\mathbf{i} = (i_1, \ldots, i_n)$ be a vector of nonnegative integers (called a multi-index), with $|\ \mathbf{i}\ |= i_1 + \cdots + i_n$, and let N be a nonnegative integer. Them the Nth order PCE of $f(x)$ can be stated in the following way

$$\hat{f}(x) = \sum_{|\mathbf{i}|=0}^{N} a_{\mathbf{i}} \Phi_{\mathbf{i}}(x),$$

where $a_{\mathbf{i}}$ denotes the unknown coefficients to be determined and $\Phi_{\mathbf{i}}$ are n dimensional orthogonal polynomials that have the maximum order N and satisfy the following relation

$$\int_{x\in\Omega} \Phi_{\mathbf{i}}(x)\Phi_{\mathbf{j}}(x)d\Gamma(x) = \delta_{ij},\ 0 \leq|\ \mathbf{i}\ |, |\ \mathbf{j}\ |\leq N,$$

where δ_{ij} is the Kronecker delta , Ω is the support, and Γ is the chosen measure. Based on the selection of Ω and Γ, different orthogonal polynomials can be obtained (such as Hermite, Laguerre, Meixner, etc.). A review and a comparison of different sampling strategies for PCE was performed in Hadigol and Doostan (2018).

2.2.7 Boosted trees and random forests

Boosted trees (BTs), also known as gradient boosting machines, were introduced by Friedman (2001) as a supervised learning method. BTs are employed in problems of supervised learning where there are several features $x^{(i)}$ that are available in the training set and are used to estimate an output variable $y^{(i)}$ and to construct a prediction model that has a form of a collection of weaker prediction models which are usually decision trees (De'ath 2007).

Random forests (RFs) represent ensemble learning methods for classification, regression, and similar tasks. They are constructed by developing an aggregate of different decision trees from the training stage and producing as output the group which is corresponds to mode of the different groups (in classification) or to mean estimation (in regression) of individual trees (Ho 1998). RFs are used to correct the decision trees' issue of overfitting to the training dataset (Hastie et al. 2001).

2.2.8 Other approaches

There are also other approaches that are less common but still deserve to be mentioned:

- Adaptive learning/active learning—a semi-supervised machine learning method in which the algorithm refers to its information sources interactively to reach the favourable outcomes for the newly generated dataset (Gorissen et al. 2010).
- Lipschitz-based surrogates—the use of Lipschitz supporting hyperplanes for function approximation in the context of surrogate assisted optimization was proposed in Zhou et al. (2016) for the purpose of enhancing the exploitation capabilities of the optimization method, while in Kudela and Matousek (2022) the Lipschitz surrogate was used to enhance the exploration abilities of the proposed algorithm.
- Non-Uniform Rational B-splines (NURBs) based models—are characterized by a collection of control points (known as the NURBs orders and knot vectors), that result in a highly flexible and robust curve definition. They can be utilized to construct sequential sampling methods that are adaptive, and give the designer the possibility to efficiently search the interesting regions of the design space (Steuben and Turner 2014).
- Genetic Programming (GP) and Symbolic Regression (SR)—GP is a method of evolutionary computation that enables computers to solve problems automatically. GP is based on an automated learning of computer programs which is founded on the Darwinian principle of survival of the fittest (Koza 1992). In SR, GP is used to construct an empirical mathematical model of the available data. The key point of SR, unlike in the regression techniques discussed above, is not to compute the weights or coefficients in order to best fit a function, but instead to find the shape of the approximate model that is constructed by the evolutionary processes.

2.3 Ensembles of surrogates and multifidelity models

Quite often there is no single class of surrogates that performs better than the other classes for various problems and the issue of selecting the best class of surrogates for the given engineering problem can itself be a challenging problem. Also, there are situations when it is impossible to experiment with multiple classes of surrogate models and select the one which has the best performance.

Ensemble of surrogates (EoS) are being used to mitigate the drawbacks of using a single surrogate model (Acar 2015; Babaei and Pan 2016). For example, adaptive sampling methods which evaluate only a single design per cycle can be used. However, this addition of a single design at a time can become inefficient if it is possible to run the simulations in parallel (Kudela 2019). This issue was addressed in Viana et al. (2010) where the authors developed a method for adding numerous designs per one optimization cycle that is based on a concurrent utilization of EoS. The beneficiality of EoS was analyzed in Song et al. (2018), where the authors provided robustness, efficiency, and accuracy requirements for various specific problems.

A related approach is to employ a mixture (or a weighted combination) of several different surrogate models. Various approaches to compute the weights can be found in the related literature—variance of individual surrogates (Zerpa et al. 2005), a global cross-validation metric (Goel et al. 2007), and error metrics (Müller and Piché 2011) are among the most prevalent. Generally, using multiple surrogates can provide us with the possibility to put more emphasis on the good surrogates while putting less priority on the bad ones as needed.

Multi-fidelity (MF) surrogate models are constructed by a combination of different fidelity models which depend on the specifics of a given problem, with the goal of reducing the high computing cost while giving accurate solutions (Yoo et al. 2020). Multi-fidelity models usually utilize High-fidelity Models (HFMs) as well as Low-fidelity Models (LFMs) to give results of comparable accuracy to surrogates which are based only on HFMs whilst providing a notable reduction in the computation related costs.

In the uncertainty propagation methods, the input of the model is characterized by some random variable. Our interests then lie in the statistics of the output of the model. The use of Monte Carlo simulations for the estimation of these statistics frequently requires numerous evaluations to produce approximations that have sufficient levels of accuracy. The use of a MF model which integrates outputs from the computationally cheap LFMs with outputs from HFMs can result in significant reductions in the runtime and give unbiased estimates of the statistics of the HFM outputs. Similar improvements in computational costs by utilizing MF models can be achieved in optimization process by using LFMs to accelerate searching or using the LFMs in combination with various adaptive correction and trust-region model management schemes (Alizadeh et al. 2020).

2.4 Overview recent advances and applications in surrogate modelling for FEM-based models

The process of constructing surrogate models often becomes intractable in problems where the input space has high dimension, due to the numerous model responses that are needed to accurately estimate the parameters of the model. To alleviate this issue (Zhou and Lu 2020) developed a novel Kriging modeling method that was fused with a dimension reduction technique. To inspect the utility of the new method, the authors used the pertinent to low cycle fatigue life of a aero-engine compressor disc, where the proposed Kriging-based method was shown to perform better than several well-known surrogate models (such as PCE and ordinary Kriging) when small sample sizes were used.

Sanchez et al. (2017) developed a new methodology for constructing surrogate models from FEM simulations, the so-called Variable Power Law meta-model. The methodology was based upon the response surface method and on a dimensional analysis, and was utilized to compute thermal models suitable for constructing preliminary designs of Multiphysics systems. Compared to traditional surrogate models, it showed an advantage by producing light, compact forms that had sufficient accuracy of prediction over a broad range of input variables (and over several orders of magnitude). Its efficiency was demonstrated on various classes of heat transfer problems, for which it gave an accurate and simple surrogate model every time, and on a aileron actuator application.

Gogu and Passieux (2013) proposed an approach for constructing efficient surrogates for high dimensional outputs combining a novel reduced basis model and a RSM. The goal of the proposed reduced basis modeling is to solve the computationally demanding problem by projecting it onto a reduced-dimensional basis which is build sequentially according to a DOE. Although this kind of a method of an order reduction may be employed as a surrogate by itself, they showed that faster response evaluations were obtained by combining this method with the RSM. The developed method constructs surrogate models based on coefficients which need only a lower number of expensive function evaluations which was enabled by the key points approach: the expensive problem (full scale) was evaluated only at a low number of important DOE points, whilst the reduced order model was employed at the other points. The strengths of the approach are illustrated on the identification problem considering orthotropic elastic constants which was based upon full field displacements and on an example of a surrogate model of a thermal field. Compared to standard surrogate models the proposed method had comparable accuracy while there was a decrease in the resolution time of the system in the DOE by almost an order of magnitude.

Jin and Jung (2016) developed a novel technique for flexible and robust surrogate modeling for finite element model updating (FEMU). They proposed a sequentially updated surrogate model that was based upon a statistical interpretation of a Kriging model. To evaluate the effectiveness of the proposed method when applied to FEMU, they performed experimental and numerical study by employing a five-story shear model of a building. They then showed both experimentally and numerically that a Kriging model utilizing the developed method could serve as a favourable substitute for the iterative FEA.

A new framework for solving high dimensional random partial differential equations (PDE) was proposed in Nabian and Meidani (2019). The considered random PDE was approximated by an ANN (deep, feed-forward, fully-connected), with either weak or strong enforcement of boundary and initial constraints. The proposed framework was mesh-free and could also deal with irregular computational domains. The correctness of the proposed method was shown on several heat conduction and diffusion problems for which numerical results were compared to the results computed by the Monte Carlo and FEM solutions. Schulz et al. (2019) introduced a numerical method for simulating Brownian polymer dynamics in a FEM framework, in which the Brownian polymer dynamics were described by stochastic PDEs driven by a white noise. To greatly improve the speed of the fitting process of the proposed method a Kriging surrogate model was used.

Nyshadham et al. (2019) compared several different surrogate models (ANNs, Kriging, response surfaces, etc.) for predicting the properties of different materials. They tested surrogate models which interpolates energies of various materials simultaneously on a data set of ten binary alloys and found that all the surrogate models agree (qualitatively) on prediction errors for the formation enthalpy, exhibiting relative errors of less than 2.5% for the considered systems. Another comparison of different surrogate models was carried out in Pavlíček et al. (2019). Kriging, ANN, and RF models were investigated on a problem of induction-assisted laser welding, which represented a rather complicated 3D problem. They also found that, if the models have properly tuned parameters, each of them can be successfully used as a surrogate for the FEM computations. Cernuda et al. (2020) presented a critical investigation of the appropriateness of different surrogate models for FEM application in the design of a suspension bushing. They compared linear SVR, RBF kernel SVR, nu SVR, generalized linear model with an elastic net, and RF surrogate models and found that RF is the most suitable among the compared surrogate models. Wang et al. (2021) devised a convolutional ANN surrogate model for accelerating screening materials and performance prediction. They showed that the proposed approach can predict the mechanical properties of a chosen collision problem with 98.63% accuracy, outperforming other techniques for surrogate modelling (SVM, RF, response surface, and ANN).

A computational method for simulations and monitoring-supported steering of tunnel boring machines in real time was introduced in Ninic et al. (2017). This strategy is combined a process-oriented 3D FEM with accompanying RNN surrogate model to recompute the parameters of the model based on the monitoring data and to give steering parameters that were continuously optimized. This hybrid FEM and surrogate model approach was compared with a strategy that was entirely based on different surrogate models, and the hybrid method proved to be superior.

Bunnell et al. (2018) studied modeling different points on a FEM for compressor blades with unique surrogates and mesh morphing. Their results showed that mesh morphing gave good performance on various tested compressor blades—the surrogate model achieved error rates lower than 5%, while providing a 96% decrease in time needed for the structural iteration of the compressor blade.

An ANN-based technique for surrogate modeling suited for a nonlinear analysis of carbon-based nanotubes was presented in Papadopoulos et al. (2018). They proposed an ANN-based equivalent beam element which was able to accurately predict high order events that were the result of size-effects that outline the properties of carbon nanotubes at the nanoscale and could be estimated only by a micro-mechanical model. They conducted various numerical experiments for wavy and straight carbon nanotubes under compression and bending, and showed that the presented methodology was able to efficiently estimate the nonlinear responses of large-scale carbon nanotube structures needing only a fraction of time for the computation when compared to a full-scale problem.

Torkzadeh et al. (2016) used a cascade ANN (feed-forward) as the surrogate model for damage detection of plate-like structures. They developed a two-stage methodology. In stage one, location of the damages in plates were analyzed by the use of the concepts of curvature-moment and curvature-moment derivative. In stage two, in order to decrease the high computational cost of updating the FEM based model while detecting damage severity, multiple damage location criterion indexes that were grounded on the structural frequency change vector were computed by the ANN, whose structure was optimized using binary version of the bat algorithm.

In a medical applications, Liang et al. (2018) used an ANN (feed-forward, fully connected) with four hidden layers to construct a surrogate model of the zero-pressure geometry of human thoracic aortas. The surrogate model was validated by a cross-validation scheme on a data set of aorta shapes from 3125 virtual patients. They have found that the computed zero-pressure geometries gave good fit with the ones generated by the method based on FEA. While the FEA-based inverse method needed hours to days to finish the computations, the surrogate model was able to output the high precision zero-pressure geometry in a second. In a similar study, Liang et al. (2018) showed the ability of surrogates based on deep neural networks to predict the aortic wall stress distributions. The surrogate model was able to predict the stress distributions fairly accurately, exhibiting average errors of only 0.49 and 0.89% in the distribution of the Von Mises stress and the peak Von Mises stress, for a fraction of the computing costs of the full FEA. Vega and Todd (2020) applied a Bayesian ANN for cost-informed decision making and structural health monitoring in miter gates. They showed that a continuous monitoring via the proposed surrogate-assisted system could result in more economical decisions with respect to maintenance policies than using only the data from visual inspections. Yet another medical application of a Kriging-based surrogate model, this time for resonance frequency analyses of dental implants, was developed in Chu et al. (2019).

Berthelson et al. (2021) used Kriging and response surface surrogate models for investigating relative injury tendencies across various conditions of a vehicular impact. The surrogate modeling approach for injury analysis demonstrated great promise, requiring only 97 high fidelity FEM simulations to evaluate a wide range of motor vehicle collision scenarios exhibiting only a nominal prediction error, which saved substantial computational time and related costs, whilst enabling a thorough analyses of the influences of various collision conditions.

In the field of biomechanical engineering, Wee et al. (2016) developed response surface-based surrogate model of the biomechanics of a bone fracture fixation that was based on high numbers of FEM simulations. The developed surrogate models displayed a good fit with the results from FEA with R^2 score that ranged from 0.62 to 0.97.

The reviewed papers on surrogate modelling are summarized in Table 5, highlighting their choice of surrogates, and theoretical and application advancements.

3 Sensitivity analysis and uncertainty quantification

Sensitivity analysis (SA) is employed to determine the effect of the input parameters on a given outcome variable (Yang et al. 2016). It is often used as the preliminary step before an early design, analysis of uncertainty, or optimization to reduce problem complexity. Testing model sensitivity is an integral part of building any mathematical or simulation models. Different values of the parameters of a model as well as the initial (input) values of variables can be subject to various sources of uncertainties. Good comprehension of the sensitivity of the outputs of the model to various uncertainties in the values of the parameters and input variables is important for strengthening our confidence in our model and the resulting predictions (Alizadeh et al. 2020).

There are currently two complementary approaches for SA—local methods, and global methods. Local methods work by perturbing the inputs of one particular design in order to approximate its partial derivatives, which give sensitivities of inputs around the chosen design. Global methods aim to determine the effect of the parameters over the entirety of the design space. With the exception of methods for fast

Table 5 Considered literature on surrogate modelling, and properties of the models

References	Surrogates						Theoretical advancement	Application
	RSM	RBF	Kriging	ANN	SVR	Other		
Gogu and Passieux (2013)	×						Reduced basis model	Structural problems
Zhang and Au (2014)			×				N/A	Cable-stayed bridge
Jin and Jung (2016)			×				Finite element model updating	Structural problems
Torkzadeh et al. (2016)				×			N/A	Damage detection
Wee et al. (2016)	×						N/A	Bone fracture fixation
Ninic et al. (2017)				×			Hybrid FEM and surrogate model	Steering of tunnel boring machines
Sanchez et al. (2017)	×						Variable Power Law meta-model	Heat transfer problems
Bunnell et al. (2018)		×	×				N/A	Compressor blades
Liang et al. (2018)				×			N/A	Aortic wall stress distribution
Liang et al. (2018)				×			N/A	Human thoracic aortas
Papadopoulos et al. (2018)				×			N/A	Carbon nanotubes
Chu et al. (2019)			×				N/A	Analysis of dental implants
Ghorbel et al. (2019)				×			Adaptive run parameterization	Fluid dynamics
Nabian and Meidani (2019)				×			Mesh-free framework for solving PDEs	Heat conduction and diffusion problems
Schulz et al. (2019)			×				Novel numerical method	Brownian polymer dynamics
Nyshadham et al. (2019)	×		×	×			Benchmarking	Binary alloys
Pavlíček et al. (2019)			×	×		×	Benchmarking	Induction-assisted laser welding
Al Kajbaf and Bensi (2020)			×	×	×		Benchmarking	Estimation of storm surge
Cernuda et al. (2020)		×			×	×	Benchmarking	Suspension bushing
Lai et al. (2020)						×	Orthogonal decomposition	Parameter estimation
Vega and Todd (2020)				×			N/A	Structural health monitoring
Zhou and Lu (2020)			×				Dimension reduction technique	Cycle fatigue of compressor disc
Asteris et al. (2021)				×			N/A	Cement mortar materials
Brown et al. (2021)				×			N/A	Fluid dynamics
Berthelson et al. (2021)	×		×				N/A	Relative injury tendencies
Jin (2021)			×				Accelerated surrogate modeling	N/A
Wang et al. (2021)	×			×	×	×	Benchmarking	Material performance
Wang et al. (2022)			×				Annealing combinable Gaussian process	N/A

parameter prescreening, the methods of global analysis are generally more computationally demanding than the local methods. As both global and local methods are based upon simulating samples, faster evaluations of surrogate models can be used to speed up the process of sample generation, which is especially useful for variance-based techniques that require numerous samples.

On the other hand, SA also plays an important part in constructing surrogate models. By employing SA, promising inputs for the surrogate model can be found, which can reduce the complexity of the model (Alizadeh et al. 2020). In problems where there is a rather complex surrogate model (such as a black-box FEM model), we can utilize SA alongside a surrogate model to get better knowledge about the behaviour of the model.

Whilst the goal of SA is the quantification of the effect of changing one input on the output, uncertainty quantification (UQ) (also called uncertainty analysis, uncertainty propagation, or reliability analysis) is used for investigating the likeliness of a change in the outputs that is induced by some uncertain inputs (Lee and Chen 2008). There has been a lot of work made to come up with methods of uncertainty quantification (UQ) in diverse fields such as stochastic mechanics, structural reliability, quality engineering, etc., and there is now a considerable number of techniques available.

The techniques for UQ can be categorized into five classes. The first class consists of the simulation-based techniques like Monte Carlo methods, and importance and adaptive sampling. The second class consists of the local expansion-based techniques such as the Taylor series expansion or perturbation techniques, which are generally weak when there is a large variability in the inputs and nonlinearities in the performance function (Lee and Chen 2008). The third class is the most probable point (MPP)-based techniques, which contain the first-order reliability methods and the second-order reliability methods. The fourth class comprises of techniques that are based on functional expansion. The PCE as well as the Neumann expansion method are found in this class. The PCE method has recently gained increased attention in stochastic mechanics, uncertainty representations, solution of stochastic differential equations, etc. The last class contains techniques that are based on numerical integration. One of the techniques in this classes is the dimension reduction technique (Rahman and Xu 2004), which works by approximating the (multidimensional) moment integrals by several (reduced-dimensional) integrals that are based upon additive decompositions of a performance function.

3.1 Overview of recent advances and applications in SA and UQ for FEM-based models

Eigel and Gruhlke (2021) developed an approach based on a domain decomposition scheme for high dimensional random PDEs which exploits the localization of the random parameters. The method uses hybrid local surrogates based on multielement generalized polynomial chaos expansion with the possibility to speed up the generation of samples by bypassing the assembly of operators and algebraic operations. They investigated the efficiency of the developed method on computational benchmark problems that illustrate the identification of nontrusted regions for sampling and trusted regions of the surrogate.

Gaspar et al. (2014) assessed the effectiveness of Kriging surrogates for problems in structural reliability which involve time-consuming nonlinear FEA models. The efficiency was investigates by systematically comparing the accuracy of the predictions of failure probability that were based on the first-order reliability methods that utilized the commonly used first-order and second-order polynomial RSM as well as Kriging models as the surrogates for the true expensive-to-compute limit state functions. They showed on a marine structures application that for structural reliability problems the Kriging models were efficient as surrogate models and, compared with the commonly used polynomial RSM, Kriging could provide substantially more accurate predictions of failure probability. This approach was further improved in Gaspar et al. (2017) by using a two-stage approach utilizing a trust region method.

In structural health monitoring, a technique for probabilistic prediction of the growth of a fatigue crack was developed in Leser et al. (2017). Prohibitive, time-consuming stress intensity factor computations were supplemented by efficient Kriging surrogate model that was trained on high-fidelity FEM simulations. Noisy visual assessments of the location history of the crack tip were utilized for the UQ of the model parameters. By utilizing the proposed surrogate modeling technique, they were able to reduce the simulation times by several orders of magnitude whilst maintaining high accuracy levels. Similar application of Kriging surrogates can be found in Su et al. (2017), where the authors developed a Monte Carlo method-based Dynamic Gaussian Process Regression surrogate for performing reliability analyses of complicated engineering structures.

Huang et al. (2016) applied a probabilistic method based on a surrogate model in the analyses of the effect of uncertainties in the process of deep drawing. They compared two types of surrogate models, quadratic response surface and Kriging, and found that Kriging models were more appropriate and accurate in modeling deep drawing processes.

The use of surrogate models has found numerous applications in the assessing the properties of composite structures. Omairey et al. (2019) developed a response surface-based multiscale surrogate model for efficient estimation of the stiffness properties of composite laminas, and also taking into account geometric and material uncertainty at laminate, meso, and micro-scale. Haeri and Fadaee (2016) proposed an advanced Kriging surrogate model for reliability analyses of laminated composites, employing a probabilistic classification function along with a metric for the refinement of the model. They demonstrated that the approach is significantly faster than using ANN-based surrogates, without sacrificing any predictive capabilities. Mukhopadhyay et al. (2016) presented the impact of noise on stochastic natural frequency analyses based on surrogate models of composite laminates. They developed an algorithm for exploring the

Table 6 Considered literature on sensitivity analysis and uncertainty quantification, and properties of the models

References	Surrogates						Theoretical advancement	Application
	RSM	RBF	Kriging	ANN	SVR	Other		
Gaspar et al. (2014)	×		×				Benchmarking	Structural reliability
Kersaudy et al. (2015)			×			×	Hybrid surrogate for UQ	Numerical dosimetry
Nobari et al. (2015)			×				N/A	Squeal noise of a real disc brake
Haeri and Fadaee (2016)			×	×			Benchmarking	Laminated composites
Huang et al. (2016)	×		×				Benchmarking	Deep drawing
Mukhopadhyay et al. (2016)			×				N/A	Composite laminate
Gaspar et al. (2017)	×		×				Two-stage approach	Structural reliability
Leser et al. (2017)			×				N/A	Structural health monitoring
Owen et al. (2017)			×			×	Benchmarking	N/A
Su et al. (2017)			×			×	Dynamic Gaussian process	Structural health monitoring
Tripathy and Bilionis (2018)				×			High dimensional UQ	Stochastic PDEs
Deng et al. (2020)						×	Drifted Wiener processes	Remaining useful lifetime prediction
Omairey et al. (2019)	×						Multiscale surrogate model	Composite laminas
Shi et al. (2019)	×						N/A	Vibration analysis
Slot et al. (2020)			×			×	N/A	Wind turbine reliability
Eigel and Gruhlke (2021)						×	Domain decomposition	N/A
Rocas et al. (2021)			×				Nonintrusive uncertainty quantification	Automotive crash problems
Wang et al. (2021)			×				Theory-guided neural network	N/A
Rocas et al. (2022)			×				Adaptive sampling methodology	Crashworthiness models
Ye et al. (2022)						×	N/A	In-stent restenosis

impact of noise in surrogate-based UQ methods and verified the approach for stochastic frequency analyses of spherical shallow shells using a surrogate model based on Kriging.

An application of Kriging-based surrogate models in vibration analyses of graphene sheets was proposed in Shi et al. (2019), conducting UQ for both Armchair and Zigzag graphene sheets. The LHS method was used to effectively propagate the uncertainty in material and geometrical features of the FEM-based model and the convergence and accuracy of the Kriging-based model were verified by comparing them with available references.

The reviewed papers on sensitivity analysis and uncertainty quantification are summarized in Table 6, highlighting their choice of surrogates, and theoretical and application advancements.

4 Surrogate-assisted optimization

The state-of-the-art in solving costly and complex problems that arise in real-world applications involves the utilization of surrogate models during optimization (Stork et al. 2020), i.e. in the search of the configuration of the design variables that produces the most desirable (optimal) outcome that is measured by a so-called objective function. The FEM-based models belong to a category of so-called black-box problems, in which the problem information that is available, such as mathematical equations and/or other exploitable knowledge of the problem is very limited, and the only method of extracting any information is the costly evaluation of the candidate designs.

The main goal of surrogate-assisted optimization (SAO) lies in the reduction of the resources, time, and the related costs by exploiting all information that is available efficiently to lower the number of objective function evaluations that are needed. Often, this is achieved by using only a few of the expensive true function evaluations to construct a "rough" surrogate model and running an optimization algorithm on this surrogate. The optimal solution from this computation is then used as a next point for another expensive true function evaluation and the refinement of the surrogate model. This process is then repeated until a stopping criterion (such as number of iteration, computational time, "good enough solution", precision of the surrogate, etc.) is met.

The optimization problems where the information about the derivative of the function is not symbolically nor numerically available are commonly categorized as derivative-free optimization (DFO) problems (Rios and Sahinidis 2013). Algorithms for DFO problems can be categorized into local search and global search methods. Local search algorithms are used to refine a solution or to reach a local optimum from an initial point. On the other hand, global search methods employ a mechanism that allows them to escape from local minima.

In the category of the local search methods are the direct search optimization algorithms that sequentially evaluate candidate points that are generated by a particular strategy (which often utilize geometric patterns), such as the Hooke and Jeeve's algorithm (Hooke and Jeeves 1961) and the Nelder-Mead (NM) method (Nelder and Mead 1965). Trust-region methods are also in the category of local search methods which use a surrogate model in a close neighbourhood of a given sample location. Another local search method is sequential quadratic programming (SQP), which at each iteration constructs a quadratic approximation of the optimization problem and finds the corresponding solution (Nocedal and Wright 2006).

In global search methods, we can find the partitioning methods such as the DIRECT algorithm (Jones et al. 1993), and stochastic algorithms. The stochastic algorithms have become especially popular for SAO in recent years (Jin et al. 2019), with methods such as simulated annealing (SiA) (Kirkpatrick et al. 1983), and evolutionary algorithms (EA) (Baeck et al. 1997) such as genetic algorithms (GA) (Goldberg and Holland 1988), particle swarm optimization (PSO) (Poli et al. 2007), differential evolution (DE) Storn and Price (1997) and many others (Matousek et al. 2022). One of the drawbacks of using stochastic algorithms is the need for proper tuning of their respective hyperparameters (Kazikova et al. 2020).

Highly challenging optimization problems are in many cases concerned with more than a single objective function. The multiple objectives (MO) are commonly aggregated into a single objective function by a weighted sum (or similar aggregation function) which makes it approachable by using ordinary (single objective) optimization methods. A different approach is to take all objectives into consideration in parallel which is particularly important if these objectives are conflicting, such as price and quality in production or drag and lift in airfoil design (Stork et al. 2020).

Although several algorithms for multi-objective SAO have already been developed, the field still lacks a repository where the different approaches could be collected and compared, because the development of these methods tends to be application-oriented and these methods have commonly been used to solve a particular real-word or industrial optimization task. Of the algorithm that are more widely used are the multiobjective genetic algorithm NSGA-II (Deb et al. 2002), the ParEGO algorithm (Knowles 2006), and the RASM method (Loshchilov et al. 2010).

As uncertainty plays a significant role in design, incorporating ways of dealing with uncertainty into the optimization process is often an important step that guarantees that the resulting optimal design can handle variations in input parameters. One possibility is to apply SA to the result obtained by the optimization process, and, if found inadequate, modifying the objective function or the constraints. Another possibility is to use robust optimization (RO), which gives a mathematical framework for optimization which is designed to minimize the propagation of the input uncertainties to the output responses (Chatterjee et al. 2019).

4.1 Overview of recent advances and applications in SAO for FEM-based models

In this subsection, we review the recent application of SAO. Table 7 gives a summary of the publications including surrogate model type, optimization methodology, and application.

4.1.1 Surrogate model types

The most ubiquitous choice of the surrogate model in applications that use surrogate-assisted optimization is Kriging, followed by RSM and ANN. Especially in the last few year, deep ANN are gaining increased popularity (Abueidda et al. 2020). Both kernel-based methods, RBF and SVR, were used only in a few applications, and PCE and RF were not used at all. GP was used by Mendes et al. (2013) and Easum et al. (2017) to build the surrogate, and in both instances the optimization was carried out by a GA. Li et al. (2019) developed a novel adaptive Singular Value Decomposition (SVD)-Krylov reduced order model as a surrogate for solving problems in structural optimization. Utilizing the SVD, they show that for a structural optimization problem the solution space of can be partitioned into a design subspace and a geometry subspace, which can be effectively approximated by a collection of different surrogate models. They show on a set of

Table 7 Considered literature on surrogate-assisted optimization, and properties of the models

References	Surrogates								Optimization			Application
	RSM	RBF	Kriging	ANN	SVR	Other	EoS	MF	MO	Uncertainty	Algorithm	
Mendes et al. (2013)						GP			×	RO	GA	Magnetostatics
Leifsson et al. (2015)	×										Trust-region	Multi-element trawl-doors
Lim et al. (2015)			×						×		Specialized	IPM synchronous motor
Tan et al. (2015)	×										PSO	Induction generator
Bramerdorfer and Zăvoianu (2017)	×			×			×		×	SA	EA	Electrical machine
Christelis et al. (2017)		×									EA	Coastal aquifers
Easum et al. (2017)	×	×				GP	×		×		GA	Patch antenna
Lal and Datta (2017)					×				×		GA	Coastal aquifers
Li et al. (2017)			×								EI	Stent and dilatation balloon
Shi et al. (2017)				×					×		GA	Ceramic heat exchanger
Shi et al. (2017)			×		×		×		×		SiA	Dental implant
Shi et al. (2017)	×										SQP	GEO satellites
Wu et al. (2017)			×								Specialized	Fluid-structure interaction
Bonfiglio et al. (2018)			×					×		UQ	EI	Supercavitating hydrofoils
Hassan et al. (2018)			×						×	SA	PSO	nanoantenna
Kaya and Hajimirza (2018)				×						SA	SiA	Organic solar cells
Liu et al. (2018)			×							UQ	PSO	Composite battery box
Park et al. (2018)			×							RO	Specialized	IPM motor
Pfrommer et al. (2018)				×							DE	Textile manufacturing
Putra et al. (2018)			×						×		EI	Stent geometry
Qin et al. (2018)			×							SA	PSO	Bridge structures
Qiu et al. (2018)	×									RO	PSO	Crashworthiness
Silber et al. (2018)				×					×		GA	Electric machines
Taran et al. (2018)			×						×		DE	Axial flux machines
Wang et al. (2018)			×						×	UQ	EI	Polymer nanocomposites
Benaouali and Kachel (2019)	×										GA	Aircraft wing
Fan et al. (2019)			×							RO	Specialized	Crane bridges
Li et al. (2019)						SVD					Specialized	Structural shape
Lin et al. (2019)		×								UQ	EA	Mooring system
Meng et al. (2019)	×									UQ	Specialized	Wind turbine blades
Rafiee and Faiz (2019)	×									RO	PSO	Outer rotor magnet

Table 7 continued

References	Surrogates								Optimization			Application
	RSM	RBF	Kriging	ANN	SVR	Other	EoS	MF	MO	Uncertainty	Algorithm	
Tan et al. (2019)			×								DE	Heat transfer coefficients
Watts et al. (2019)	×									SA	Specialized	Multiscale topology
White et al. (2019)				×							Specialized	Multiscale topology
Xu et al. (2019)			×								Specialized	Wind turbine blade
Yong et al. (2019)			×					×		SA	EI	Whole engine models
Zhao et al. (2019)				×					×		GA	Viscous damper system
Abueidda et al. (2020)				×						SA	Specialized	Topology of 2D structures
Bouhlel et al. (2020)	×			×			×				SQP	Airfoil shape
Dong et al. (2020)				×							NM	Elastic metamaterials
Qian et al. (2020)	×										GA	Engineering design
Tie et al. (2020)		×								RO	Specialized	CFPR laminates
Yan et al. (2020)					×						GA	Aero-engine turbine
Yoo et al. (2020)		×						×	×	UQ	GA	Composite structures
Fatahi (2021)			×						×	SA	GA	Welded plates
Ktari et al. (2021)	×								×		Specialized	Ring tensile specimen

numerical examples that the proposed methodology exhibits performance gains when compared to most already existing heuristic techniques.

The use of EoS and MF models is also not as wide-spread as one would expect, given their advantageous properties. EoS were used in conjunction with MO problems in Bramerdorfer and Zăvoianu (2017), where the authors used different global and local surrogate models for optimizing electric machine design, in Easum et al. (2017), where the EoS based method performed better than the traditional NSGA-II on a optimization of a patch antenna design, and in the design of dental implants in Shi et al. (2017). Bayesian optimization was used in maximizing the EI of MF surrogates for a realistic large-scale hydrostructural optimization of 3D supercavitating hydrofoils in Bonfiglio et al. (2018). MF surrogates were also used for solving realistic design problems concerning whole gas turbine engines Yong et al. (2019) and reliability-based optimization of various composite structures (Yoo et al. 2020).

4.1.2 Optimization models and algorithms

The consideration of multiple objective in FEM-based optimization problems is relatively widespread, appearing in around a third of the considered publications. The multiple objective have various forms depending on the particular application and are frequently connected to buckling load and structural mass in structural design applications (Yoo et al. 2020), response reduction ratio and value of a damping force in damper systems (Zhao et al. 2019), wall shear stress and initial average stress in stent geometry optimization (Putra et al. 2018), gain, front-to-back ratio, and ground plane area for patch antenna design (Easum et al. 2017), etc.

Almost a half of the considered publications included some form of dealing with uncertainty in the optimization model. UQ was frequently used together with the Kriging surrogate in Bonfiglio et al. (2018), Liu et al. (2018), and Wang et al. (2018). Applications utilizing SA frequently used ANN (Bramerdorfer and Zăvoianu 2017; Kaya and Hajimirza 2018; Abueidda et al. 2020) or Kriging (Hassan et al. 2018; Qin et al. 2018; Yong et al. 2019; Fatahi 2021) surrogates.

Stochastic optimization methods, be it SiA or evolutionary approaches (EA, GA, PSO), were the algorithm of choice for more than a half of the considered publications, which might be attributed to their relatively low implementation complexity and satisfactory performance. More interestingly, a growing number of authors used a specialized algorithm in their applications. Wu et al. (2017) used the surrogate management framework algorithm Booker et al. (1998), a mesh-based method that contains two strategies: a surrogate model as a tool for prediction to facilitate global exploration and to identify promising regions, and the use a local grid search or similar pattern-search techniques to guarantee convergence at least to local minima. Park et al. (2018) proposed a robust optimization method that uses a sub-domain Kriging to decrease the memory allocations during the optimization and a gradient-free sensitivity index, that measures the sensitivity of the fitness function value to the input variables. Meng et al. (2019) used collaborative optimization method based on uncertainties, which is a bi-level multidiscipline design optimization method, to approach the turbine blades design problem and to improve its aerodynamic performance.

4.1.3 Application areas

The employment SAO has permeated into a wide range of applied areas. In electrical engineering, these models are now quite routinely used to aid the design of IPM (Interior Permanent Magnet) motors (Lim et al. 2015; Park et al. 2018; Rafiee and Faiz 2019) and axial flux machines (Taran et al. 2018), induction generators (Tan et al. 2015), composite battery boxes (Liu et al. 2018), all-electric GEO satellites (Shi et al. 2017), or antennas (Easum et al. 2017; Hassan et al. 2018). Also ubiquitous are mechanical engineering applications, which include the design of wind turbine blades (Meng et al. 2019; Xu et al. 2019), aero-engine turbines (Yan et al. 2020), viscous damper systems (Zhao et al. 2019), welded plates (Fatahi 2021), ring tensile specimens (Ktari et al. 2021), or whole engine models (Yong et al. 2019), and civil engineering applications of topology optimization (Qin et al. 2018; White et al. 2019; Fan et al. 2019; Li et al. 2019; Abueidda et al. 2020).

Recently, SAO has been used in maritime applications. Leifsson et al. (2015) performed shape optimization of multi-element trawl-doors, which are for many fishing vessels the major contributors to their fuel expenditure, as they may be responsible for approximately 10–30% of the total drag of the vessel. Lin et al. (2019) presented a scantling optimization of a common internal turret area for mooring system of floating production storage and offloading units, which constitute some of the most widely used production platforms in offshore oil production. They report on achieving a weight reduction of 10.2%, computed by a SAO utilizing the RBF surrogate model and an EA. Lal and Datta (2017) investigated the viability and efficiency of utilizing artificial freshwater recharge in order to increase the pumping of fresh groundwater from wells. They used a SVR as a surrogate for the expensive simulations and a multi-objective GA for finding optimal solutions for recharge and integrated pumping, and for maintaining the levels of saltwater intrusion in the coastal aquifer within acceptable limits. Similar problem was investigated in Christelis et al. (2017), where the authors used the RBF surrogate and a single objective formulation solved by an EA instead. Their results demonstrated an outperformance of the SAO methods against the direct optimization, as their method located the best solutions and demonstrated a robust performance for all optimization problems of coastal aquifer management.

Shi et al. (2017) developed a geometric model of a ceramic microchannel heat exchanger which included the heat transfer channel, the inlet part, and outlet part and conducted a numerical study to enhance the uniformity of the fluid flow. Then the authors constructed a radial basis neural network surrogate model and optimized the heat exchanger design using a GA. At the optimal design point, they report that the nonuniformity of the fluid flow was decreased by 68.2% and pressure drop has increased by 6.6%, which results in a significant improvement in the uniformity of the fluid flow in the heat exchanger with just a little cost of pressure drop. Another thermal engineering application can be found in Tan et al. (2019), where the authors used the Kriging surrogate and the DE algorithm to compute more accurate convective heat transfer coefficients in thermal analysis of spindle. They compared the results of the simulation temperatures using the optimized convective heat transfer coefficients with the experimental temperatures and found that they agreed well exhibiting the absolute error of the simulation not exceeding 0.5 °C and the relative error of the simulation not exceeding 2.34%.

Simple UQ method for evaluating numerical uncertainty as well as surrogate uncertainty in a crashworthiness optimization process was proposed in Qiu et al. (2018). They showed that the conventionally used 95% confidence interval was insufficient for obtaining robust results especially when encountering high levels of noise in the simulations because the commonly used number of samples for building surrogates is too small for reaching accurate estimates of the noise level.

Kaya and Hajimirza (2018) demonstrated that surrogates can be utilized for accurate predictions of the optical properties of thin solar cells and even for the optimization their structures. Instead of the time-consuming finite difference time domain methods for computing optical properties of arrangements at small sub-wavelength scales, they designed a two-layer ANN surrogate model for estimating the optical absorptivity of the cell. They then used a combination of steepest descend and SiA for the optimization of the cell parameters. The solutions found by SAO demonstrated enhancement factors that were higher than 270% for the optical absorptivity.

The use of SAO is also becoming more common in medical applications. Design optimization of stents and its dilation balloons, which are used in treating cardiovascular diseases, has investigated in Li et al. (2017). By using a Kriging surrogate and SAO, they were able to refine the fatigue life and expansion performance of both diamond-shaped and sv-shaped stents. Stent geometry was also the focus of Putra et al. (2018). SAO with expected hypervolume improvement and Kriging method were used to construct the surrogate model and to find the best configuration of parameters to the intravascular hemodynamics of the stent. In Shi et al. (2017) the authors used EoS and SAO in a dental application to reduce stress at the implant-bone interface to improve the implantation success rate by using the structure optimization of dental implant with other characteristics of dental implant only slightly deteriorating or optimizing simultaneously.

SAO also found recent applications in identifying interphase properties the properties in polymer nanocomposites (Wang et al. 2018), optimizing elastic metamaterial structures (Dong et al. 2020), optimizing manufacturing process parameters using deep ANN (Pfrommer et al. 2018), or maximizing the impact-resistance of patch repaired carbon fiber reinforced polymer laminates (Tie et al. 2020).

5 Software tools

As the employment of surrogates for analyzing and optimizing computationally expensive problems have become more prevalent, new software tools that provide an easy access to the needed technologies emerged. Few of the most used and recently developed software tools are listed below in alphabetical order:

- *ALAMO* (Cozad et al. 2014): ALAMO (Automated learning of algebraic models for optimization) is a methodology for classification and regression that aims to build accurate and simple surrogates based on a minimal collection of datapoints. It uses a technique based on integer programming to select from a high number of input variables and their possible transformations.
- *ARGONAUT* (Boukouvala and Floudas 2017): ARGONAUT is a framework designed to deal with DFO problems with either a total or a partial lack of closed form or analytical expressions for objective function or constraints. Pivotal feature of this framework is also surrogate model selection in which the surrogate models are selected from a library of regression models (including linear, quadratic and polynomial RSM) which are straightforward to optimize and various interpolation models (including RBF and Kriging) that have better data prediction accuracy.
- *Agros Suite and Ārtap* (Karban et al. 2021): Agros Suite is an environment for numerically solving second order PDEs by a higher-order FEM with a variety of other advanced features, including various optimization techniques and full adaptivity. Ārtap, a Python toolbox for robust design optimization provides an efficient and simple programming environment that encompases a broad-range of integrated as well as external PDE solvers,

optimization methods and well-known machine learning techniques for building surrogate models.

- *Eureqa* (Schmidt and Lipson 2009): Eureqa is a software (commercially available) for building surrogate models. Its procedures start with the initial data set and follow by computing symbolic regressions in which the search is not only bounded to the coefficients but also to regression model forms as well (similar to GP). It then constructs a collection of candidate regression models, where the precision of the models is evaluated by computing symbolic differentiation of the models and by comparing their derivatives with the initial dataset. On the basis of these computations, the models are sequentially recomputed until a convergence criterion is met.
- *FReeT* (Novak and Novak 2018): FReeT (Feasible Reliability Engineering Tool) is a multipurpose probabilistic software for reliability and sensitivity analysis of various problems in engineering, with incorporated PCE surrogate modelling enabling sensitivity and reliability analysis.
- *MATLAB toolboxes*: MATLAB has a dedicated Statistics and machine learning toolbox which supports subset selection employing goodness-of-fit measures, linear and nonlinear regression, regularization, and SVR. Validation metrics for studying the performance of classification algorithms, non-parametric regression algorithms and surrogates, are also included.
- *MATSuMoTo* (Mueller 2014): MATSuMoTo is the MATLAB Surrogate Model Toolbox for black-box, computationally expensive, global optimization problems, which offers various choices for initial experimental design strategies, sampling strategies, surrogate models and surrogate model mixtures. MATSuMoTo can also compute several function evaluations in parallel by utilizing the Parallel Computing Toolbox available in MATLAB.
- *Python toolboxes*: One of the options in Python is the SMT toolbox (Bouhlel et al. 2019), which contains several surrogate modelling methods, PyDOE toolbox offers a collection of different static sampling methods, and the well-known ScikitLearn (Pedregosa et al. 2011), Tensorflow (Abadi et al. 2016) and PyTorch (Paszke et al. 2017) all contain different model validation schemes and surrogate model types.
- *RBFOpt* (Costa and Nannicini 2018): RBFOpt is an open-source library for optimizing a black-box function over a mixed-integer box-constrained set. The algorithm is based on the RBF surrogate and performs a fast procedure for automatic model selection.
- *Surrogate Modeling (SUMO) Toolbox* (Gorissen et al. 2010): SUMO is a MATLAB toolbox for adaptive sampling and surrogate modeling which offers several surrogate model choices (Kriging, SVM, ANN, etc.), model selection algorithms, DOE methods, sample evaluation methods, and optimization algorithms (PSO, EI, SiA, GA, etc.).
- *Surrogates Toolbox* (Viana and Goel 2010): Another general purpose MATLAB toolbox for building surrogate models which contains several third-party software packages and has four primary capabilities: DOE, surrogate model construction (Kriging, RBF, etc.), model validation, and optimization along with sensitivity analysis.
- *SurroOpt* (Han 2016): SurroOpt is a research code developed for engineering designs and academic research guided by expensive numerical simulations. A notable feature is that constructing the surrogate and solving optimization problems that correspond to the infill-sampling criteria are looked at as new optimization mechanisms, the role of which is the same as any of the normal gradient-based techniques or stochastic optimization algorithms.

6 Trends, research gaps, and practical recommendations

The presented review affirms that surrogate modelling is a well grounded methodology in current research of FEM-based analysis and optimization of various systems. Performance and sensitivity analysis, uncertainty quantification, and also surrogate assisted design optimization become more accessible, mainly because of the huge reductions in computational costs. In the following text, we discuss the practical aspects and application trends that were extracted from the considered literature.

- The usefulness of surrogate models is mainly connected to the reduction in computational resources and time needed for certain analyses whilst keeping high accuracy levels. Even though there exist many examples showing advantageous use of surrogate models for UQ and SA, there still remains a gap in the knowledge on the extent of achievable time savings. The time savings were thoroughly analysed primarily in papers dealing with SAO.
- Researchers have been searching for more generalized surrogates that could be applied to various dissimilar problems. Multiple publications investigated the maximum capabilities of single surrogates, while the focus on the automation of the process of deriving surrogates (such as in ALAMO), and the employment of EoS or MF models is still underutilized.
- Most types of surrogate models have low interpretability of the underlying mathematical structures and, as such, are ill suited for answering any analytical questions.
- A common issue is the restricted number of design variables that surrogate models can deal with without suffering prohibitive computational cost. To this end, it

became popular to incorporate sensitivity analysis to the process of the derivation of the surrogate model to find the parameters that are most important. Dimension reduction techniques are also becoming popular for reducing the number of considered inputs.
- The proper choice of the initial sampling scheme is also uncertain. Most of the reviewed papers used LHS.
- In the cases where the size of the problem is higher, the required accuracy levels are lower, while the time for computations remains unchanged, RBF and RSM seem to be the appropriate choice of surrogates. Kriging is a method that displays in high accuracy levels and relatively good performance for larger problem sizes, but is not well suited for problems that have more than roughly 50 variables. For high-dimensional problems, SVM performs well even with high levels of nonlinearity.
- For SA and UQ, the most widely used surrogates in recent applications were Kriging and PCE.
- Using off-the-shelf optimization algorithms, such as NSGA-II, for finding the optimal surrogate-based design is a common practice, but building an application-oriented method can bring significant improvements.
- There now exists a wide range of readily available software tools for both building and validating surrogate models, and for SAO.

7 Conclusion

Surrogate models are becoming increasingly more and more utilized in multiple scientific and engineering disciplines and found applications in various fields. On the other hand, the selection of the appropriate surrogate for the given problem is not straightforward due to various trade-offs that are associated with using the different surrogates. This choice is a bit clearer if the given problem can be classified as model building/prediction, sensitivity analysis or uncertainty quantification, or optimization. The differences in the various techniques for every one of these categories from point of view of surrogate modeling were reviewed and relevant current advances and new applications in the different categories were investigated with the focus on surrogates. There now exist several software tools that give the user an easy entry to the techniques that were investigated in this paper. These tools were mentioned with a short explanation of their respective aims and capabilities.

We anticipate, that future research in surrogate models for FEM-based computations will focus more on developing automated tools for selection and construction of surrogates, as well as an efficient use of EoS and MF models, based on where in the three classes the particular application is located. We also expect future analyses to concentrate further on decreasing computational cost related to deriving surrogate models and on improving their interpretability.

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Declarations

Conflict of interest We confirm that this manuscript is the authors’ own original work, has not been published and is not under consideration for publication elsewhere. We declare that the authors have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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