Calibration Experimental Design Considering Field Response and Model Uncertainty

Zhen Hu, Dan Ao, Sankaran Mahadevan¹
Department of Civil and Environmental Engineering
Vanderbilt University, Nashville, TN, 37235

Abstract

Calibration experiment design optimization (CEDO) seeks to identify the optimal values of experimental inputs in order to maximize the obtained information within testing budget constraints. Current CEDO methods only consider observation errors and focus on problems with low-dimensional response variables. This paper proposes a new robust CEDO model for Bayesian calibration with field response and incorporates various sources of model uncertainty such as surrogate model uncertainty, numerical discretization error, and model discrepancy, into CEDO. Since sampling-based methods to estimate the posterior distributions and thus compute the objective function (information gain) are computationally expensive, this paper develops an analytical method to estimate the objective function while accounting for model uncertainty during this process. Based on the evaluation of objective function, a global sensitivity analysis (GSA)-based method is proposed to check the quality of surrogate models used in CEDO, guide the training and improvement of the surrogate models, and thus reduce the effect of surrogate model uncertainty on CEDO. The optimal experimental input settings are obtained using the efficient global optimization (EGO) method. A nonlinear analytical example and a heat transfer example are used to illustrate the effectiveness of the proposed approach.

Keywords: Model calibration; Bayesian approach; Kullback-Leibler (K-L) divergence; Optimization; Experimental Design; Sensitivity Analysis;

¹Corresponding author, Box 1831, Station B, Vanderbilt University, Nashville, Tennessee, 37235, USA. Tel.: +1-615-322-3040, E-mail: sankaran.mahadevan@vanderbilt.edu.

1. Introduction

Calibration experiment design optimization (CEDO) is the process of determining the optimal values of experiment settings expected to yield the most valuable observation data for model calibration [1]. Collecting observation data from experiments for complicated systems is often very costly [2]. In this situation, experiments optimally designed for the purpose of model calibration can significantly reduce the economic cost, by achieving the desired calibration accuracy and confidence with fewer experiments.

During the past decades, experimental design methods for Bayesian model calibration have been investigated for linear models [3] and empirical models [4, 5]. These simplifications and assumptions simplified the experimental design problems. The results obtained based on these simplifications, however, may be sub-optimal and sometimes may be useless since the simplified model is quite different from the true model. Motivated by overcoming these drawbacks, a group of experimental design optimization methods have been developed for systems with nonlinear response by taking advantage of recently developed advanced simulation techniques. For instance, Huan and Marzouk [2, 6] proposed Bayesian experimental design methods using information-theoretic measures and gradient-based stochastic optimization techniques; Long et. al. [7, 8] proposed efficient computation of the expected information gain using Laplace approximations; and Ryan et. al. [9] presented a simulation-based approach for experimental design for a small number of design variables. The above reviewed experimental design optimization methods provide rigorous frameworks for experimental design optimization; however, they have three main limitations that are sought to be overcome in this paper.

First, current methods mainly focus on problems with a single response variable or low-dimensional response variables even if the observations may be high-dimensional due to multiple

experimental settings. But in some situations, the observation data are collected from field response, such as temperature, pressure, or deformation values observed at multiple locations in a test specimen [10]. A challenge in CEDO with field response is how to efficiently construct surrogate models to substitute the computationally expensive high-fidelity simulation models. Building a single surrogate model for the field response can be inaccurate since the optimal characteristics for one output may not be the same as for the others [11]. Training many independent surrogate models one for each location may be another way, but the correlation between responses cannot be considered. Co-kriging [12] might be a third way of addressing this issue, but current co-kriging approaches appear to be limited to low-dimensional outputs.

Second, only observation errors are considered in current CEDO methods. As an important source of uncertainty, model uncertainty which includes surrogate model uncertainty, discretization error, and model discrepancy, sometimes is more dominant than observation errors in practical situations. Note that CEDO has to be done before actual testing and therefore with synthetic data, which are typically generated from the simulation model by including observation error during the optimization. The simulation model used for the experimental design is not yet calibrated (since the experiments are not performed yet); thus it may not correctly represent the original response of the system and may have significant discrepancy from the original response. The surrogate model used to substitute for the simulation model may also not correctly represent the original simulation model due to the limited number of training points; at untrained points, the surrogate model has prediction uncertainty. Due to the involvement of various sources of model uncertainty, the optimal design obtained from CEDO may not be the real optimal. How to effectively include various sources of model uncertainty along with the observation errors within CEDO is a critical issue that needs to be solved.

Third, amongst various sources of model uncertainty, some of them are reducible during CEDO. For example, the surrogate model uncertainty can be reduced by adding more training points. However, without a rigorous way of quantifying the effects of various sources of model uncertainty on the experiment design, we will not know whether the surrogate models are good enough for CEDO and when should we stop adding new training points. In addition, how to efficiently solve the CEDO model is also a challenge that needs to be solved.

In this paper, we propose a new framework for CEDO with field response in the presence of the various sources of model uncertainty and observation errors. A new robust CEDO model is formulated by considering both the expectation and variance of Kullback-Leibler (K-L) divergence in the objective function. In order to address the problem of surrogate modeling, the singular value decomposition (SVD) [13] based Kriging surrogate modeling method implemented by Jia et. al. [11], and Hombal and Mahadevan [14] for output prediction, and the low-rank data compression method developed in Refs. [15-17], are extended to CEDO with field response. Based on the surrogate modeling method, modeling of various sources of model uncertainty in CEDO is studied. In order to efficiently solve the CEDO model, an analytical way of solving the objective function is developed based on the Fisher information matrix [7, 18]. Since some of the model uncertainty is reducible, a global sensitivity analysis-based method is proposed to check the quality of the surrogate model. Based on the above efforts, the efficient global optimization (EGO) method [19] is employed to solve the optimization problem. The contributions of this paper can thus be summarized as: (1) a framework for experimental design optimization in the presence of surrogate model uncertainty, model discrepancy, and numerical discretization error, (2) integration of dimension reduction techniques with surrogate modeling to handle high-dimensional field response during CEDO, (3) an efficient way of computing the

objective function (information gain) in the presence of various sources of model uncertainty, (4) a way of checking the quality of the surrogate modeling for CEDO, and (5) a solution procedure for the resulting new robust CEDO formulation.

The rest of the paper is organized as follows. We first provide a brief background on model calibration under uncertainty and CEDO in Section 2. Section 3 presents the proposed methodology. A numerical example and a heat transfer example are provided in Section 4 to demonstrate the proposed method. Section 5 provides the conclusions.

2. Problem statement

In this section, we briefly review background regarding Bayesian calibration and CEDO.

2.1. Model calibration under uncertainty

Let $\mathbf{x} = [x_1, x_2, \dots, x_{n_x}]^T$ be the input variables of a model G and $\boldsymbol{\theta} = [\theta_1, \theta_2, \dots, \theta_{n_\theta}]^T$ be the parameters that need to be calibrated. Consider a single scalar physical quantity of interest y , the simulation model output y_s , which is the prediction of y , is given by

$$y_s = G(\mathbf{x}, \boldsymbol{\theta}). \quad (1)$$

Denoting the corresponding observation from experiments as y_{obs} , and using the Kennedy O'Hagan (KOH) framework [20], we have

$$y_{obs}(\mathbf{x}, \boldsymbol{\theta}) = y(\mathbf{x}, \boldsymbol{\theta}) + e_{obs}, \quad (2)$$

$$y(\mathbf{x}, \boldsymbol{\theta}) = y_s(\mathbf{x}, \boldsymbol{\theta}) + e_{FEA}(\mathbf{x}, \boldsymbol{\theta}) + d(\mathbf{x}, \boldsymbol{\theta}), \quad (3)$$

where e_{obs} is the observation error, $d(\mathbf{x}, \boldsymbol{\theta})$ is the model discrepancy term which represents uncertainty due to model inadequacy, and $e_{FEA}(\mathbf{x}, \boldsymbol{\theta})$ is the numerical discretization error of the

simulation model. e_{obs} is usually treated as a zero-mean Gaussian random variable. Note that the values of $\mathbf{x}$ are chosen by the experimenter, while $\boldsymbol{\theta}$ take some unknown deterministic values $\boldsymbol{\theta}^{true}$ during the experiments.

Combining Eqs. (1) through (3), we have

$$y_{obs}(\mathbf{x}, \boldsymbol{\theta}) = G(\mathbf{x}, \boldsymbol{\theta}) + d(\mathbf{x}, \boldsymbol{\theta}) + e_{FEA}(\mathbf{x}, \boldsymbol{\theta}) + e_{obs}. \quad (4)$$

Assume that n_{obs} observation data of y_{obs} are collected from experiments with input variables $\mathbf{x}^{(1)}, \mathbf{L}, \mathbf{x}^{(n_{obs})}$, where $\mathbf{x}^{(i)}$ are the input settings for the i -th experiment. Denoting the observation data as $\mathbf{y}_{obs} = [y_{obs}^{(1)}, y_{obs}^{(2)}, \mathbf{L}, y_{obs}^{(n_{obs})}]^T$, the joint posterior distribution of $\boldsymbol{\theta}$ is computed using Bayes' theorem as [20]

$$\boldsymbol{\pi}_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs}) = \frac{L(\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x}^{(1)}, \mathbf{L}, \mathbf{x}^{(n_{obs})}) \boldsymbol{\pi}_0(\boldsymbol{\theta})}{\int_{\mathbf{W}_\theta} L(\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x}^{(1)}, \mathbf{L}, \mathbf{x}^{(n_{obs})}) \boldsymbol{\pi}_0(\boldsymbol{\theta}) d\boldsymbol{\theta}}, \quad (5)$$

where $\mathbf{W}_\theta$ is the domain of $\boldsymbol{\theta}$, $\boldsymbol{\pi}_0(\boldsymbol{\theta})$ is the joint prior distribution of $\boldsymbol{\theta}$, $L(\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x}^{(1)}, \mathbf{L}, \mathbf{x}^{(n_{obs})})$ is the likelihood function, and $\boldsymbol{\pi}_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs})$ is the joint posterior distribution.

2.2. Calibration experimental design optimization (CEDO)

Eq. (5) indicates that the posterior distributions of $\boldsymbol{\theta}$ are affected by the quality of the collected observation data $\mathbf{y}_{obs}$, which are governed by the input variables $\mathbf{x}$ of the experiments. For some problems, we may have limited resources to perform experiments. Due to the limited resources, determining the optimal experimental settings of inputs $\mathbf{x}$ to collect the most valuable observations becomes very important.

Calibration experimental design optimization (CEDO) seeks to maximize the information gain from the experiments for model calibration under uncertainty. In this paper, the information

gain is measured using the Kullback-Leibler (K-L) divergence from the posterior distribution to the prior distribution. For given experimental input settings $\mathbf{x}$ and the corresponding experimental observation $\mathbf{y}_{obs}$, the K-L divergence of $\boldsymbol{\theta}$ is given by [3, 21]

$$D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) = \int_{\mathcal{W}} \pi_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs}, \mathbf{x}) \log \frac{\pi_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs}, \mathbf{x})}{\pi_0(\boldsymbol{\theta})} d\boldsymbol{\theta}. \quad (6)$$

From Eq. (4), it can be seen that the observation $\mathbf{y}_{obs}$ is uncertain for given experiment settings $\mathbf{x}$ and value of $\boldsymbol{\theta}$, due to d , e_{FEA} , and e_{obs} . In order to account for the uncertainty in $\mathbf{y}_{obs}$, the expected value of K-L divergence can be used in CEDO, and is given by [6]

$$F(\mathbf{x}) = \int_{\mathcal{W}} \int_{\mathcal{W}} D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) p(\mathbf{y}_{obs} | \boldsymbol{\theta}) d\mathbf{y}_{obs} \pi_0(\boldsymbol{\theta}) d\boldsymbol{\theta} = E_{\boldsymbol{\theta}}(E_{\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))), \quad (7)$$

where $p(\mathbf{y}_{obs} | \boldsymbol{\theta})$ is the probability density function (PDF) of observations conditioned on $\boldsymbol{\theta}$, $E_{\boldsymbol{\theta}}(\cdot)$ is to account for the uncertainty in $\boldsymbol{\theta}$ and $E_{\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x}}(\cdot)$ is to consider the uncertainty in $\mathbf{y}_{obs}$ for given $\boldsymbol{\theta}$ and $\mathbf{x}$, and $\mathcal{W}$ is the domain of response $\mathbf{y}_{obs}$.

Based on the expected K-L divergence, an unconstraint design optimization model can be formulated to determine the optimal experimental input settings:

$$\max_{\mathbf{x}} \{F(\mathbf{x})\} \quad \text{s.t. } \mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u], \quad (8)$$

where $\mathbf{x}_l$ and $\mathbf{x}_u$ are the lower and upper bounds of the design variables $\mathbf{x}$, respectively.

Methods have been developed in recent years to determine the optimal experimental input settings for Bayesian calibration. As discussed in Section 1, current methods mainly focus on single or low-dimensional response variables [2, 6], and do not include model uncertainty. Note that $\mathbf{y}_{obs}$ can also be high-dimensional for a single response variable, due to a large number of experiments. However, that case is different from the focus of this paper which is high-dimensional field response even from one experiment. Since solving Eq. (8) will evaluate the

simulation model $G(\mathbf{x}, \boldsymbol{\theta})$ more than thousands of times, a surrogate model $\hat{G}(\mathbf{x}, \boldsymbol{\theta})$ is often used to substitute an expensive simulation model $G(\mathbf{x}, \boldsymbol{\theta})$ in Bayesian calibration. The use of surrogate models and simulation models introduces various sources of model uncertainty in CEDO, which need to be included in the design. In the following section, we develop a new CEDO method for problems with field response and accounting for model uncertainty.

3. Proposed methodology

In this section, we first formulate the new CEDO model with high-dimensional field response. Following that, we will discuss how to solve the optimization model.

3.1. Robust CEDO with high-dimensional field response

In practical experiments, sometimes the experimental observation of the output for a given value of input $\mathbf{x}$ is not a single value, but a field response. Or in other words, for a given input setting $\mathbf{x}$, we will obtain $\mathbf{y}_{obs} = [y_{obs}(\mathbf{z}^{(1)}), \dots, y_{obs}(\mathbf{z}^{(n_z)})]$ from one experiment, where $\mathbf{z}^{(i)}$ is the i -th observation location and n_z is the number of observation locations. After introducing the observation coordinate into the simulation model, Eqs. (1) is rewritten as

$$\mathbf{y}_s(\mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = [y_s(\mathbf{z}^{(1)}, \mathbf{x}, \boldsymbol{\theta}), \dots, y_s(\mathbf{z}^{(n_z)}, \mathbf{x}, \boldsymbol{\theta})]^T = G(\mathbf{x}, \boldsymbol{\theta}), \mathbf{z} \hat{\mathbf{I}} \mathbf{W}_z \quad (9)$$

in which $y_s(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) = G(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}), \mathbf{z}^{(i)} \hat{\mathbf{I}} \mathbf{W}_z$.

Similarly, Eq. (4) is rewritten as

$$\begin{aligned} y_{obs}(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) &= y_s(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + d(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + e_{FEA}(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + e_{obs}(\mathbf{z}^{(i)}), \\ &= G(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + d(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + e_{FEA}(\mathbf{z}^{(i)}, \mathbf{x}, \boldsymbol{\theta}) + e_{obs}(\mathbf{z}^{(i)}), \mathbf{z}^{(i)} \hat{\mathbf{I}} \mathbf{W}_z, \end{aligned} \quad (10)$$

where $\mathbf{W}_z$ is the spatial domain (locations) of the response.

In the formulation of the new CEDO model, the high-dimensional response needs to be considered. Besides, the current CEDO models only focus on maximizing the expected value of

K-L divergence as indicated in Eqs. (7) and (8). Only accounting for the expected value of K-L divergence, however, may not give us a robust experimental design since the uncertainty in $\mathbf{y}_{obs} = [y_{obs}(\mathbf{z}^{(1)}, \mathbf{x}, \boldsymbol{\theta}), L, y_{obs}(\mathbf{z}^{(n_z)}, \mathbf{x}, \boldsymbol{\theta})]$ results in the uncertainty in $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})$. In this paper, the new CEDO model is formulated as a robust design optimization problem [22]. In the new CEDO model, the expected value of K-L divergence is maximized while the variance is minimized. The maximization of the expected value is to obtain the optimal experimental settings and the minimization of the variance is to improve the robustness of the design.

Based on the above discussion, the new CEDO model is defined for problems with field response as follows

$$\begin{aligned} \min_{\mathbf{x}} F(\mathbf{x}) &= \{w_1 s_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) - w_2 E_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))\}, \\ \text{s.t. } \mathbf{x} &\in [\mathbf{x}_l, \mathbf{x}_u], \end{aligned} \quad (11)$$

where $0 \leq w_1 \leq 1$ and $0 \leq w_2 \leq 1$ are user-specified weights for mean and standard deviation of the objective, $w_1 + w_2 = 1$, and $E_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ and $s_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ are given by

$$\begin{aligned} E_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) &= \int_{\mathbb{W}_0} \int_{\mathbb{W}_1} \int_{\mathbb{W}_2} D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) f(\mathbf{y}_{obs}|\mathbf{x}, \boldsymbol{\theta}) dy_{obs}(\mathbf{z}^{(1)}, \mathbf{x}, \boldsymbol{\theta}) L \\ &\quad dy_{obs}(\mathbf{z}^{(n_z)}, \mathbf{x}, \boldsymbol{\theta}) \pi_0(\boldsymbol{\theta}) d\boldsymbol{\theta}, \quad \mathbf{z}^{(1)}, L, \mathbf{z}^{(n_z)} \in \mathbb{W}_2; \boldsymbol{\theta} \in \mathbb{W}_0, \end{aligned} \quad (12)$$

and

$$\begin{aligned} s_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}^2(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) &= \int_{\mathbb{W}_0} \int_{\mathbb{W}_1} \int_{\mathbb{W}_2} [D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) - E_{\mathbf{y}_{obs}|\boldsymbol{\theta}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))]^2 f(\mathbf{y}_{obs}|\mathbf{x}, \boldsymbol{\theta}) \\ &\quad dy_{obs}(\mathbf{z}^{(1)}, \mathbf{x}, \boldsymbol{\theta}) L dy_{obs}(\mathbf{z}^{(n_z)}, \mathbf{x}, \boldsymbol{\theta}) \pi_0(\boldsymbol{\theta}) d\boldsymbol{\theta}, \quad \mathbf{z}^{(1)}, L, \mathbf{z}^{(n_z)} \in \mathbb{W}_2; \boldsymbol{\theta} \in \mathbb{W}_0, \end{aligned} \quad (13)$$

where $f(\mathbf{y}_{obs}|\mathbf{x}, \boldsymbol{\theta})$ is the joint PDF of $\mathbf{y}_{obs} = [y_{obs}(\mathbf{z}^{(1)}, \mathbf{x}, \boldsymbol{\theta}), L, y_{obs}(\mathbf{z}^{(n_z)}, \mathbf{x}, \boldsymbol{\theta})]$ for given $\boldsymbol{\theta}$ and $\mathbf{x}$. Note that the above equation is just for one observation of the field response. It can also be extended for multiple observations. Eq. (11) is one way to formulate the multi-objective

optimization problem. Other approaches can be considered alternatively, such as e -constraint method, goal programming etc.

There are three main challenges explained as below for solving the above CEDO model.

(1) *Surrogate modeling*: The response function needs to be evaluated thousands of times during CEDO, which is very computationally expensive. Surrogate models are widely used in Bayesian calibration to substitute the original response function as discussed in Sec. 2.1. For problems with field response, directly constructing a surrogate model is not applicable since it may lead to large errors [11]. Besides, constructing a single surrogate model for the high-dimensional response is computationally expensive as matrices with large amounts of data need to be processed repeatedly during the modeling and prediction of the surrogate model.

(2) *Evaluation of the objective function*: For problems with high-dimensional field response, the model uncertainty is also high-dimensional and correlated over space. This raises two issues. The first one is how to properly quantify the high-dimensional model uncertainty. The second one is how to efficiently and effectively estimate the objective function by incorporating various sources of model uncertainty into the calibration experimental design.

(3) *Optimization*: Even if the challenges one and two are solved, directly solving the optimization model given in Eq. (11) is still computationally expensive. How to efficiently solve Eq. (11) is also a challenge.

In the subsequent sections, we will discuss how to solve the above three challenges.

3.2. Surrogate modeling of high-dimensional field response

In this paper, the Kriging method briefly summarized in Appendix A is used for the surrogate modeling. However, we do not construct a surrogate model directly for the high-dimensional field response. The high-dimensional field response is first mapped into low-dimensional latent

responses using data compression techniques. The surrogate model is then constructed in the latent space using the Kriging approach.

3.2.1. Data compression of high-dimensional response

Denoting the high-dimensional spatial observation data as $s(\mathbf{z}, \mathbf{d}) : \Omega_z \times \Psi \rightarrow \mathbb{R}$ over a spatial domain $\mathbf{W}_z$ and design domain Ψ , where $\mathbf{z}$ is the spatial location and $\mathbf{d}$ stands for a specific realization in the design domain. Suppose there are n_z locations over the spatial domain $\mathbf{W}_z$ and n_d different realizations in the design domain, we then have the observation data matrix as follows:

$$\begin{aligned} \mathbf{s} &= [\mathbf{s}(\mathbf{d}^{(1)}), \mathbf{s}(\mathbf{d}^{(2)}), \dots, \mathbf{s}(\mathbf{d}^{(n_d)})] \in \mathbb{R}^{n_z \times n_d} \\ &= \{[s(\mathbf{z}^{(i)}, \mathbf{d}^{(j)})]\}, \forall i = 1, 2, \dots, n_z; j = 1, 2, \dots, n_d, \end{aligned} \quad (14)$$

where $\mathbf{s}(\mathbf{d}^{(j)}) = [s(\mathbf{z}^{(1)}, \mathbf{d}^{(j)}), s(\mathbf{z}^{(2)}, \mathbf{d}^{(j)}), \dots, s(\mathbf{z}^{(n_z)}, \mathbf{d}^{(j)})]^T$ and $\mathbf{z}^{(i)}, i = 1, 2, \dots, n_z$ is the i -th observation location.

The observation data matrix $\mathbf{s}$ can be decomposed by singular value decomposition (SVD) [23] or eigenvalue decomposition (EVD) to facilitate the surrogate modeling. Since the SVD method can be applied to non-square matrices whereas EVD is only defined for square matrices, the SVD method is employed here. With the SVD method, $\mathbf{s}$ is then decomposed as [24]

$$\mathbf{s} = \mathbf{W}\mathbf{H}\mathbf{V}^T, \quad (15)$$

where $\mathbf{W} \in \mathbb{R}^{n_z \times n_z}$ is an orthogonal matrix, $\mathbf{H} \in \mathbb{R}^{n_z \times n_d}$ is a rectangular diagonal matrix, and $\mathbf{V} \in \mathbb{R}^{n_d \times n_d}$. The diagonal elements of $\mathbf{H}$ are the singular values $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \dots, \lambda_{n^*}]$, where $n^* = \min(n_d, n_z)$, arranged in decreasing order.

Based on the decomposition, we then define another matrix as $\boldsymbol{\beta} = \mathbf{H}_r \mathbf{V}_r^T$, where $\mathbf{H}_r \in \mathbb{R}^{n_z \times r}$ contains the r -biggest singular value of $\mathbf{H}$ and $\mathbf{V}_r \in \mathbb{R}^{n_d \times r}$ contains the first r columns of $\mathbf{V}$ [15,

25, 26] and define $\mathbf{W}_r \in \mathbb{R}^{n_z \times r}$, which contains the first r columns of $\mathbf{W}$. The original data matrix is then compressed as

$$\mathbf{s}(\mathbf{d}^{(j)}) \approx \sum_{i=1}^r b(i, j) \boldsymbol{\phi}_i, \quad j = 1, 2, \dots, n_d, \quad (16)$$

where $b(i, j)$ is the element of $\hat{\boldsymbol{\beta}} \hat{\mathbf{I}}^{-1} \mathbf{r}^{n_d}$ at i -th row and j -th column, $\boldsymbol{\phi}_i$ is the i -th column of $\mathbf{W}_r$, which represents the j -th important feature used to approximate $\mathbf{s}$. The number of important features r is determined based on the magnitude of singular value and $r \ll k$.

Based on the above compression, the high-dimensional field response data matrix $\mathbf{s}$ is mapped into low-dimensional latent response $\boldsymbol{\beta}$. For some problems, the above discussed compression method may not be applicable because a large matrix of $\mathbf{s} \hat{\mathbf{I}}^{-1} \mathbf{r}^{n_d}$ has a high requirement of computer memory and computational time. In this situation, a *low-rank data compression method* presented in Ref. [15-17] can be employed.

The basic idea of the low-rank data compression method is to perform a truncated SVD for n_1 stochastic realizations $\mathbf{s}^{temp} \in \mathbb{R}^{n_z \times n_1}$ first. Denote the obtained truncated singular value matrix, eigenvector matrix, and orthogonal matrix as $\mathbf{W}_r^{temp} \in \mathbb{R}^{n_z \times r}$, $\mathbf{H}_r^{temp} \hat{\mathbf{I}}^{-1} \mathbf{r}^{r}$, and $\mathbf{V}_r^{temp} \hat{\mathbf{I}}^{-1} \mathbf{r}^{n_1 \times r}$. We have $\mathbf{s}^{temp} \approx \mathbf{W}_r^{temp} \mathbf{H}_r^{temp} (\mathbf{V}_r^{temp})^T$. When n_{new} new observations (new designs) are obtained, we perform truncated SVD for the new observations and have $\mathbf{s}^{new} \approx \mathbf{W}_r^{new} \mathbf{H}_r^{new} (\mathbf{V}_r^{new})^T$, where $\mathbf{W}_r^{new} \in \mathbb{R}^{n_z \times r}$, $\mathbf{H}_r^{new} \hat{\mathbf{I}}^{-1} \mathbf{r}^{r}$, and $\mathbf{V}_r^{new} \hat{\mathbf{I}}^{-1} \mathbf{r}^{n_{new} \times r}$. $\mathbf{W}_r^{temp}$, $\mathbf{H}_r^{temp}$, $\mathbf{V}_r^{temp}$ and $\mathbf{W}_r^{new}$, $\mathbf{H}_r^{new}$, $\mathbf{V}_r^{new}$ are then used to formulate two concatenated matrices such that $\mathbf{A} := [\mathbf{W}_r^{temp} \mathbf{H}_r^{temp} \quad \mathbf{W}_r^{new} \mathbf{H}_r^{new}] \in \mathbb{R}^{n_z \times 2r}$ and $\mathbf{B}^T = \begin{bmatrix} (\mathbf{V}_r^{temp})^T & \mathbf{0} \\ \mathbf{0} & (\mathbf{V}_r^{new})^T \end{bmatrix} \in \mathbb{R}^{2r \times (n_1 + n_{new})}$. It can be seen that $\mathbf{A}$ and $\mathbf{B}^T$ have rank $2r$. Then the reduced QR-factorization method [15] is used to convert the rank $2r$ matrix into rank r matrix

and thus obtain the updated $\mathbf{W}_r$, $\mathbf{H}_r$, $\mathbf{V}_r$, based on which the high-dimensional response is compressed into low dimensional latent responses using Eq. (16). More details and the algorithms for low-rank data compression can be found in Ref. [15-17]. Note that $\mathbf{s}^{temp}$ and $\mathbf{s}^{new}$ are much smaller than $\mathbf{s}$. By using the low-rank data compression, the requirement of memory is reduced [15-17]. Next, the Kriging approach is employed for the surrogate modeling based on the data compression.

3.2.2. Kriging surrogate model based on data compression

In CEDO, the input variables of the surrogate model include not only the experimental input settings $\mathbf{x} \in \mathbb{R}^{n_x}$, but also the calibration parameters $\boldsymbol{\theta}$ since $\boldsymbol{\theta}$ are unknown and the response function needs to be evaluated with different values of $\boldsymbol{\theta}$. The output is the observation variable of the high-dimensional field response in experiments. In order to integrate the Kriging model with data compression for surrogate modeling of the high-dimensional field response, training points are first generated for design variables. Denote the training points as $\mathbf{d} = [\mathbf{d}^{(1)}, \mathbf{d}^{(2)}, \dots, \mathbf{d}^{(n_t)}]$, where $\mathbf{d}^{(i)} = [\mathbf{x}^{(i)}, \boldsymbol{\theta}^{(i)}]$ is the i -th training point, $\mathbf{x}^{(i)}$ and $\boldsymbol{\theta}^{(i)}$ are corresponding training points of $\mathbf{x}$ and $\boldsymbol{\theta}$, and n_t is the number of training points. For each training point $\mathbf{d}^{(i)}$, a field response is obtained as below using the simulation model:

$$\mathbf{y}_s(\mathbf{z}, \mathbf{d}^{(i)}) = [y_s(\mathbf{z}^{(1)}, \mathbf{d}^{(i)}), \dots, y_s(\mathbf{z}^{(n_z)}, \mathbf{d}^{(i)})]^T = G(\mathbf{x}^{(i)}, \boldsymbol{\theta}^{(i)}), \quad \mathbf{z} \in \mathbb{R}^{n_z}, \quad (17)$$

where $y_s(\mathbf{z}^{(j)}, \mathbf{d}^{(i)})$ stands for the simulation response at observation location $\mathbf{z}^{(j)}$ with the i -th training point $\mathbf{d}^{(i)} = [\mathbf{x}^{(i)}, \boldsymbol{\theta}^{(i)}]$ as the input settings to the simulation model $G(\mathbf{x}, \boldsymbol{\theta})$.

After performing simulations at all the training points, a data matrix is obtained for the response field as follows

$$\mathbf{y}^s = [\mathbf{y}_s(\mathbf{z}, \mathbf{d}^{(1)}), \mathbf{y}_s(\mathbf{z}, \mathbf{d}^{(2)}), \dots, \mathbf{y}_s(\mathbf{z}, \mathbf{d}^{(n_t)})] \in \mathbb{R}^{n_z \times n_t}. \quad (18)$$

Eq. (18) can be further written as

$$\mathbf{y}^s = \left\{ \left[y_s(\mathbf{z}^{(i)}, \mathbf{d}^{(j)}) \right] \right\}, \forall i = 1, 2, \dots, n_z; j = 1, 2, \dots, n_t. \quad (19)$$

Note that the above matrix is obtained by reshaping the spatial responses at each training point into a one-dimensional array (i.e. $\mathbf{y}_s(\mathbf{z}, \mathbf{d}^{(i)}) = [y_s(\mathbf{z}^{(1)}, \mathbf{d}^{(i)}), y_s(\mathbf{z}^{(2)}, \mathbf{d}^{(i)}), \dots, y_s(\mathbf{z}^{(n_z)}, \mathbf{d}^{(i)})]^T$ denotes all the observation location responses at i -th training point). After the reshaping of the matrix, the field response $\mathbf{y}^s$ at all the training points becomes a data matrix in the form shown in Eq. (14).

To reduce the dimensionality of the random field response, the data compression method is employed next as discussed in Section 3.2.1. Define the decomposition matrices obtained from data compression as $\mathbf{W}_r$, $\mathbf{H}_r$, and $\mathbf{V}_r$, the data matrix in Eq. (19) is reconstructed as

$$y_s(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) \approx \sum_{k=1}^r b_k(\mathbf{d}^{(i)}) j_k(\mathbf{z}^{(j)}), \quad i = 1, 2, \dots, n_t; j = 1, 2, \dots, n_z, \quad (20)$$

where $b_k(\mathbf{d}^{(i)})$ is obtained based on $\mathbf{H}_r$ and $\mathbf{V}_r$ using the method presented in Sec. 3.2.1 and $j_k(\mathbf{z}^{(j)})$ is element of $\mathbf{W}_r$ at the j -th row and k -th column. Note that, the above equation is also a kind of representation of random field, which is similar as the Karhunen-Loeve expansion.

From Eq. (20), it can be seen that the coefficient vector $b_k(\mathbf{d}^{(i)})$ is different for different training points, whereas $\boldsymbol{\phi}_k = [j_k(\mathbf{z}^{(1)}), j_k(\mathbf{z}^{(2)}), \dots, j_k(\mathbf{z}^{(n_z)})]^T$, $k = 1, 2, \dots, r$, are independent of the training points. $b_k(\mathbf{d}^{(i)})$ represents the coefficient of k -th feature $\boldsymbol{\phi}_k$ at realization $\mathbf{d}^{(i)}$. It means that the variation in the random field response mainly comes from the change in $b_k(\mathbf{d}^{(i)})$. The dimensionality of $b_k(\mathbf{d}^{(i)})$ is usually much lower than that of the original field response. Here, $b_k(\mathbf{d}^{(i)})$, $k = 1, 2, \dots, r$, are not the original responses; we call them the latent responses.

With all the training points $\mathbf{d}^{(i)}$ and $b_k(\mathbf{d}^{(i)})$, $k = 1, 2, \dots, r$, at corresponding training points, we then construct surrogate models for $b_1(\mathbf{d})$, $b_2(\mathbf{d})$, $\dots$, and $b_r(\mathbf{d})$ using the Kriging method as discussed in Appendix A. After that, Eq. (20) becomes

$$\hat{y}_s(\mathbf{z}, \mathbf{d}) \approx \sum_{j=1}^r \hat{b}_j(\mathbf{d}) j_j(\mathbf{z}), \quad \mathbf{z} \in W_Z, \mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u], \text{ and } \boldsymbol{\theta} \in W_\theta, \quad (21)$$

where $\mathbf{d} = [\mathbf{x}, \boldsymbol{\theta}]$ and $\hat{b}_j(\mathbf{d})$ represents the surrogate model of the j -th hidden response, $b_j(\mathbf{d})$.

Until now, we have discussed how to construct a surrogate model to substitute for $G(\mathbf{x}, \boldsymbol{\theta})$ with high-dimensional field response. In the following section, we will study how the surrogate model is applied to CEDO.

3.3. Model uncertainty in CEDO

Current experimental design methods only consider observation errors [6]. In this section, we first analyze the sources of model uncertainty in calibration. After that, we investigate the effect of model uncertainty on CEDO.

3.3.1. Sources of model uncertainty in CEDO

The model uncertainty in calibration mainly comes from three sources as indicated in Fig. 1, which are summarized as below:

- *Surrogate model uncertainty:* (a) Surrogate model bias: In the SVD-based Kriging surrogate model (Sec. 3.2.2), the first r important features are used to reconstruct the original high-dimensional response. Due to the truncation of important features, the SVD-based Kriging surrogate model has bias from the original response of the simulation model. (b) Surrogate model prediction uncertainty: There is uncertainty in the prediction with a surrogate model at untrained prediction points.

Fig. 1 Model uncertainty sources in CEDO

- *Model discrepancy of physics simulation model:* Model discrepancy is also called model bias or model inadequacy [20]. It stems from both missing physics (model form error) in the simulation model. In the commonly used Kennedy and O’Hagan (KOH) [20] framework for Bayesian model calibration, the model discrepancy term is modeled as an input-dependent Gaussian process [27]. For problems with high-dimensional field response, the application of the KOH framework is not straightforward. The model discrepancy term of the high-dimensional response is also high-dimensional. In that case, the Gaussian process cannot be built directly for the discrepancy term. A possible solution for this is to extend the KOH framework based on the data compression-based Kriging surrogate method presented in the last section.

- *Numerical discretization error:* Using a discretization method such as finite element or finite difference methods to numerically solve differential equations have been widely used in current engineering simulation models. The coarse discretization of the domain introduces numerical discretization error in the physical model prediction, thus affecting the experimental design optimization. During the past decades, a group of posterior error estimation methods [28] have been proposed to estimate the discretization error in boundary value problems in mechanics, such as the posterior error estimation method proposed by Szabo [29, 30], the explicit error estimation methods [31], recovery based methods [32], and extrapolation methods [33, 34]. A detailed review of a posteriori error estimation has been provided by Ainsworth and

Oden [35]. In this paper, for the sake of illustration, the simple Richardson extrapolation method [33, 34] is used. It should be noted that there are some limitations and drawbacks for the Richardson extrapolation method [33, 34]. The Richardson extrapolation method can be easily replaced with more advanced posterior error estimation methods if desired in the proposed framework. The current focus of this paper is to investigate how to perform CEDO in the presence of various sources of model uncertainty.

Next, we will discuss how to quantify various sources of model uncertainty in CEDO.

3.3.2. Quantification of model uncertainty

(a) Surrogate model uncertainty

- Bias of surrogate model due to truncation of important features

For a training point $\mathbf{d}^{(i)}$, $i = 1, 2, \dots, n_t$ at an observation location $\mathbf{z}^{(j)}$, $j = 1, 2, \dots, n_z$, the bias of the SVD-based Kriging model due to the truncation of important features is computed by

$$d_b(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) = y_s(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) - \hat{y}_s(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}), \quad i = 1, 2, \dots, n_t; j = 1, 2, \dots, n_z. \quad (22)$$

A typical way for the modeling of bias is to build a surrogate model for the bias term [36]. Building a surrogate model for the bias is equivalent to increasing the number of important features in the surrogate modeling of $\hat{y}_s(\mathbf{z}, \mathbf{d})$. In this paper, we therefore assume the bias term as a constant at a specific observation location and use the expected bias as the constant. For an observation location $\mathbf{z}^{(j)}$, the expected bias of the surrogate model is given by

$$\bar{d}_b(\mathbf{z}^{(j)}) = \frac{1}{n_t} \sum_{i=1}^{n_t} d_b(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) / n_t, \quad j = 1, 2, \dots, n_z. \quad (23)$$

The bias term due to the truncation of important features will become negligible when a large number of important features are included in the surrogate model.

- Surrogate model prediction uncertainty

Surrogate model prediction uncertainty comes from the interpolation uncertainty of the Kriging model. For any untrained point $\mathbf{d} = [\mathbf{x}, \boldsymbol{\theta}]$, according to the property of Kriging model, we have $\hat{b}_j(\mathbf{d}) \sim N(m_{b_j}(\mathbf{d}), s_{b_j}^2(\mathbf{d}))$, where $m_{b_j}(\mathbf{d})$ and $s_{b_j}^2(\mathbf{d})$ are obtained from the surrogate model as given in Eqs. (A4) and (A6) and $N(m, s^2)$ is normal distribution. The surrogate model uncertainty of the SVD-based Kriging model at untrained point $\mathbf{d}$ and observation location $\mathbf{z}^{(i)}$ is then given by $\hat{y}_s(\mathbf{z}^{(i)}, \mathbf{d}) \sim N(m_y(\mathbf{z}^{(i)}, \mathbf{d}), s_y^2(\mathbf{z}^{(i)}, \mathbf{d}))$, in which

$$m_y(\mathbf{z}^{(i)}, \mathbf{d}) = \hat{\mathbf{a}}^r m_{b_j}(\mathbf{d}) j_j(\mathbf{z}^{(i)}), \quad (24)$$

where $m_{b_j}(\mathbf{d})$ is the mean prediction of the surrogate model $\hat{b}_j(\mathbf{d})$, and

$$s_y(\mathbf{z}^{(i)}, \mathbf{d}) = \sqrt{\hat{\mathbf{a}}^r s_{b_j}^2(\mathbf{d}) j_j^2(\mathbf{z}^{(i)})}. \quad (25)$$

(b) Numerical discretization error

As discussed in Sec. 3.3.1, the Richardson extrapolation method [33, 34] is employed to quantify the discretization error in this paper. For a given training point $\mathbf{d}^{(i)}$, $i = 1, 2, \dots, n_t$, the discretization error of the results $y_s^{(j)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)})$, $j = 1, 2, \dots, n_z$, of an FEA simulation with mesh size h_1 can be quantified based on two more FEA simulations with finer mesh size h_2 and finest mesh size h_3 as follows [33, 34]

$$e_{FEA}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) = \frac{y_s^{(1)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) - y_s^{(2)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)})}{r_{mesh}^{p_c} - 1}, \quad (26)$$

where $y_s^{(k)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)})$ is the result at location $\mathbf{z}^{(j)}$ of FEA simulation with inputs $\mathbf{d}^{(i)}$ and mesh size h_k , $r_{mesh} = h_2 / h_1 = h_3 / h_2$ is the mesh refinement ratio, and the convergence p_c is estimated as $p_c = \ln[(y_s^{(3)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) - y_s^{(2)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)})) / (y_s^{(2)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}) - y_s^{(1)}(\mathbf{z}^{(j)}, \mathbf{d}^{(i)}))] / \ln r_{mesh}$.

Due to the field response, the discretization error is also a field response. In order to account for the numerical discretization error during experimental design, we also build a surrogate model for the numerical discretization error term using the method presented in Sec. 3.2. From the surrogate model, we will have

$$\hat{e}_{FEA}(\mathbf{z}, \mathbf{d}) \approx \sum_{j=1}^{r_e} \hat{b}_{e,j}(\mathbf{d}) j_{e,j}(\mathbf{z}), \quad \mathbf{z} \in W_Z, \mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u], \text{ and } \boldsymbol{\theta} \in W_\theta, \quad (27)$$

where r_e is the number of important features used in the numerical discretization surrogate model, $j_{e,j}(\mathbf{z})$, $j = 1, 2, \dots, r_e$, is the j -th important feature of the numerical discretization term, and $\hat{b}_{e,j}(\mathbf{d})$ is the Kriging surrogate model of the SVD coefficients. Similar to the surrogate model of the simulation model, we can also obtain the bias of the discretization error surrogate model, $\hat{e}_e(\mathbf{z})$, using the method given in Sec. 3.3.2 (a).

(c) Model discrepancy for problems with high-dimensional response

The modeling of model discrepancy is only possible when the experimental design is performed adaptively. In that case, observation data will be collected from previous experiments. With available observations, the model discrepancy term of the simulation model can be included in the KOH framework. For given $\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}$, the model discrepancy is obtained by comparing the simulation model and the numerical discretization error with observation data as

$$d(\mathbf{z}, \mathbf{d}^{(i)}) = y(\mathbf{z}, \mathbf{d}^{(i)}) - y_s(\mathbf{z}, \mathbf{d}^{(i)}) - e_{FEA}(\mathbf{z}, \mathbf{d}^{(i)}), \quad i = 1, 2, \dots, n_f, \quad (28)$$

where $\mathbf{d}^{(i)} = [\mathbf{x}^{(i)}, \boldsymbol{\theta}]$, $\mathbf{x}^{(i)}$ is the input of the i -th experiment, and n_f is the number of groups of available observation data (since the response is field response).

A surrogate model can then be built for the model discrepancy term. Since the field response is high-dimensional, the discrepancy term is also high-dimensional. The surrogate model $\hat{d}(\mathbf{z}, \mathbf{d})$ can then be constructed using the surrogate modeling method presented in Sec. 3.2.1 as

$$\hat{d}(\mathbf{z}, \mathbf{d}) = \sum_{j=1}^{r_d} \hat{b}_{dj}(\mathbf{d}) j_{dj}(\mathbf{z}), \quad (29)$$

where $\hat{b}_{dj}(\mathbf{d})$ is the surrogate model of the j -th latent response, r_d is the number of important features used for the SVD of model discrepancy, and $j_{dj}(\mathbf{z})$ is the j -th important feature at location $\mathbf{z}$. Note that the hyper-parameters of $\hat{b}_{dj}(\mathbf{d})$, $j = 1, 2, \dots, r_d$, and $j_{dj}(\mathbf{z})$, $j = 1, 2, \dots, r_d$ all depend on the values of calibration parameters $\boldsymbol{\theta}$. For the sake of illustration, we denote the hyper-parameters of model discrepancy surrogate model as $\boldsymbol{\chi}^d$.

We do not know the value of the calibration parameters $\boldsymbol{\theta}$. One way of dealing with the model discrepancy term is to calibrate the hyper-parameters and other parameters which are dependent on $\boldsymbol{\theta}$ along with the calibration parameters [20]. Since the joint probability function of the calibration parameters and the $\boldsymbol{\theta}$ -dependent parameters is highly intractable and integrating out the $\boldsymbol{\theta}$ -dependent parameters is computationally expensive, Kennedy and O'Hagan [20] proposed a two-stage strategy to estimate the hyper-parameters of the surrogate model of model discrepancy term. Here, we briefly discuss how to extend the two-stage strategy to the representation of model discrepancy in high-dimensional field response.

In the first stage, a surrogate model is built for the high-dimensional response using the method given in Sec. 3.2. In the second stage, for given values of calibration parameters $\boldsymbol{\theta}$ and $\boldsymbol{\chi}^d$, the experimental response after considering the model discrepancy is given by

$$Y_{obs} | \boldsymbol{\theta}, \boldsymbol{\chi}^d = \hat{y}_s(\mathbf{z}, \mathbf{d}) + \hat{e}_{FEA}(\mathbf{z}, \mathbf{d}) + \hat{d}(\mathbf{z}, \mathbf{d}) + \mathcal{A}_b(\mathbf{z}) + \mathcal{A}_e(\mathbf{z}) + e_{obs}. \quad (30)$$

The mean and covariance function of the experimental response are given by

$$m_{y_{obs}}(\mathbf{z}^{(i)}|\mathbf{d}) = \boldsymbol{\mu}_b(\mathbf{d})\boldsymbol{\phi}(\mathbf{z}^{(i)})^T + \boldsymbol{\mu}_{b_e}(\mathbf{d})\boldsymbol{\phi}_e(\mathbf{z}^{(i)})^T + \boldsymbol{\mu}_{b_d}(\mathbf{d})\boldsymbol{\phi}_d(\mathbf{z}^{(i)})^T + \delta_b^2(\mathbf{z}^{(i)}) + \delta_e^2(\mathbf{z}^{(i)}), \quad (31)$$

and

$$\begin{aligned} Cov(Y_{obs}(\mathbf{z}^{(i)}, \mathbf{d}), Y_{obs}(\mathbf{z}^{(j)}, \mathbf{d})) = & \sum_{k=1}^{r_b} j_k(\mathbf{z}^{(i)})j_k(\mathbf{z}^{(j)})s_{b_k}^2(\mathbf{d}) + \sum_{k=1}^{r_e} j_{e,k}(\mathbf{z}^{(i)})j_{e,k}(\mathbf{z}^{(j)})s_{b_{e,k}}^2(\mathbf{d}) \\ & + \sum_{k=1}^{r_d} j_{dk}(\mathbf{z}^{(i)})j_{dk}(\mathbf{z}^{(j)})s_{b_{d,k}}^2(\mathbf{d}) + I(i, j)s_{e_{obs}}^2, \end{aligned} \quad (32)$$

where $\boldsymbol{\mu}_{b_d}(\mathbf{d}) = [m_{b_{d,1}}(\mathbf{d}), m_{b_{d,2}}(\mathbf{d}), \dots, m_{b_{d,r_d}}(\mathbf{d})]$, $s_{b_{d,k}}^2(\mathbf{d})$ is the variance of $\hat{b}_{dk}(\mathbf{d})$ prediction,

$I(i, j) = 1$, if $i = j$, otherwise $I(i, j) = 0$, and $Cov(Y_{obs}(\mathbf{z}^{(i)}, \mathbf{d}), Y_{obs}(\mathbf{z}^{(j)}, \mathbf{d}))$ is the covariance between $Y_{obs}(\mathbf{z}^{(i)}, \mathbf{d})$ and $Y_{obs}(\mathbf{z}^{(j)}, \mathbf{d})$.

Since $m_{y_{obs}}(\mathbf{z}^{(i)}|\mathbf{d})$ and $Cov(Y_{obs}(\mathbf{z}^{(i)}, \mathbf{d}), Y_{obs}(\mathbf{z}^{(j)}, \mathbf{d}))$ depend on $\boldsymbol{\theta}$ and $\boldsymbol{\chi}^d$, following the KOH procedure, the above equations are integrated with respect to the prior distribution of $\boldsymbol{\theta}$. After the integration, the mean and variance become functions of experimental inputs $\mathbf{x}$ and location variables $\mathbf{z}$ conditioned on $\boldsymbol{\chi}^d$ [20]. The hyper-parameters $\boldsymbol{\chi}^d$ of Eq. (25) can then be estimated by maximizing the likelihood function based on available observation data. After $\boldsymbol{\chi}^d$ is obtained, the hyper-parameters of the model-discrepancy term is fixed at the maximum likelihood estimate (MLE). In general, for problems with high-dimensional response, the model discrepancy term can be represented as a Gaussian random field based on available observations.

After substituting the original response model in Eq. (4) with a surrogate model plus the bias of surrogate model plus the surrogate model of the numerical discretization error plus the bias of numerical discretization error surrogate model, and the model discrepancy surrogate model if it is available, we have

$$Y_{obs}(\mathbf{z}) = \sum_{j=1}^r \hat{\mathbf{a}}_j \hat{b}_j(\mathbf{d}) j_j(\mathbf{z}) + \sum_{j=1}^{r_d} \hat{\mathbf{a}}_{dj} \hat{b}_{dj}(\mathbf{d}) j_{dj}(\mathbf{z}) + \sum_{j=1}^{r_e} \hat{\mathbf{a}}_{e,j} \hat{b}_{e,j}(\mathbf{d}) j_{e,j}(\mathbf{z}) + \mathcal{A}_b^0(\mathbf{z}) + \mathcal{A}_e^0(\mathbf{z}) + e_{obs}(\mathbf{z}). \quad (33)$$

Note that for the sake of illustration, the upper case letter $Y_{obs}(\mathbf{z})$ is used in the above equation to represent the observation which is uncertain. Subsequently in this paper, we use $Y_{obs}(\mathbf{z})$ to denote the random variable of observation and $y_{obs}(\mathbf{z})$ to represent a realization of this random variable. Considering that the biases (i.e. $\mathcal{A}_b^0(\mathbf{z})$ and $\mathcal{A}_e^0(\mathbf{z})$) due to the truncation of importance features are negligible, we omit these symbols from the subsequent equations for the sake of illustration.

3.3.3. Effect of model uncertainty on CEDO

The CEDO model given in Eq. (11) is for problems when the *original model* is used for experimental design. In that situation, the uncertainty of $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})$ only comes from the observation error and the uncertainty in priors of $\boldsymbol{\theta}$. Due to the use of simulation models and surrogate models, extra model uncertainty sources are introduced into CEDO as discussed in the above sections.

Fig. 2 depicts the effect of model uncertainty on CEDO. It shows that extra random variables $\hat{\boldsymbol{\beta}}(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d})$, and $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$ are introduced in the CEDO model after considering model uncertainty.

The CEDO model given in Eq. (11) is therefore rewritten as follows

$$\begin{aligned} \min_{\mathbf{x}} F(\mathbf{x}) = & \{w_1 S_{\hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) \\ & - w_2 E_{\hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))\}, \\ \text{s.t. } \mathbf{x} \in & [\mathbf{x}_l, \mathbf{x}_u], \end{aligned} \quad (34)$$

where $\mathbf{y}_{obs}$ is conditioned on $\boldsymbol{\theta}$, $\mathbf{x}$, $\hat{\boldsymbol{\beta}}(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$, and $\boldsymbol{\varepsilon}_{obs}$.

Note, in the above equation, $\hat{\boldsymbol{\beta}}(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d})$, and $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$ are random variables conditioned on $\boldsymbol{\theta}$.

The most critical part of solving Eq. (34) is how to efficiently estimate $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})$ for given

$\boldsymbol{\theta} = \boldsymbol{\theta}^*$, $\hat{\boldsymbol{\beta}}(\mathbf{d}) = \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*)$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d}) = \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*)$, $\hat{\boldsymbol{\beta}}_e(\mathbf{d}) = \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*)$, and $\boldsymbol{\varepsilon}_{obs} = \boldsymbol{\varepsilon}_{obs}^*$, where $\mathbf{d}^* = [\mathbf{x}, \boldsymbol{\theta}^*]$. In

the subsequent section, we will develop an efficient way to estimate the objective function.

Fig. 2. Effect of model uncertainty on CEDO ($\hat{\boldsymbol{\beta}}(\mathbf{d}) = \hat{b}_j(\mathbf{d})$, $j = 1, 2, L, r$; $\hat{\boldsymbol{\beta}}_d(\mathbf{d}) = \hat{b}_{dj}(\mathbf{d})$, $j = 1, 2, L, r_d$; and $\hat{\boldsymbol{\beta}}_e(\mathbf{d}) = \hat{b}_{ej}(\mathbf{d})$, $j = 1, 2, L, r_e$)

3.4. Solution of the objective function

3.4.1. Estimation of $D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) | \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\varepsilon}_{obs}^*$

In order to estimate $D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) | \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\varepsilon}_{obs}^*$, the posterior distribution $\pi_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs}, \mathbf{x}, \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\varepsilon}_{obs}^*)$ of the calibration parameters $\boldsymbol{\theta}$ needs to be obtained first.

(a) Estimation of $\pi_{post}(\boldsymbol{\theta} | \mathbf{y}_{obs}, \mathbf{x}, \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\varepsilon}_{obs}^*)$

A straightforward way of obtaining the posterior distributions with given observation $\mathbf{y}_{obs}$ is to use the Markov Chain Monte Carlo (MCMC) [37] or Particle Filter (PF) techniques [38]. However, the MCMC or PF-based methods are very computationally expensive when they are

applied in CEDO since CEDO needs to obtain the posterior distributions under a number of different situations. Besides, the MCMC and PF-based method will have large statistical errors when the number of samples is not large enough.

When a specific θ^* is used to generate synthetic observation data $\mathbf{y}_{obs}$ for model calibration, it has been proved that the posterior distributions can be approximated as a multivariate normal distribution, if the number of observations is larger than 10 [7, 18]. This situation holds for model calibration with a high-dimensional field response since a large number of observation data are obtained from the field response as discussed in Sec. 3.2. Based on this, the posterior distributions are given by

$$\pi_{post}(\theta | \mathbf{y}_{obs}, \mathbf{x}, \theta^*, \hat{\beta}^*(\mathbf{d}^*), \hat{\beta}_d^*(\mathbf{d}^*), \hat{\beta}_e^*(\mathbf{d}^*), \epsilon_{obs}^*) \sim N(\theta^*, \hat{\mathbf{I}}(\mathbf{y}_{obs})^{-1}), \quad (35)$$

in which $\hat{\mathbf{I}}(\mathbf{y}_{obs})$ is the Fisher information matrix [18]. The (i, j) -th element of $\hat{\mathbf{I}}(\mathbf{y}_{obs})$ is given by

$$\hat{I}_{ij}(\mathbf{y}_{obs}) = - \frac{\partial^2}{\partial \theta_i \partial \theta_j} \log(L(\mathbf{y}_{obs}, \mathbf{x})) \bigg|_{\theta = \theta^*, \hat{\beta}(\mathbf{d}) = \hat{\beta}^*(\mathbf{d}^*), \hat{\beta}_d(\mathbf{d}) = \hat{\beta}_d^*(\mathbf{d}^*), \hat{\beta}_e(\mathbf{d}) = \hat{\beta}_e^*(\mathbf{d}^*)}, \quad i, j = 1, 2, \dots, n_q, \quad (36)$$

where $L(\mathbf{y}_{obs}, \mathbf{x}) = L(\mathbf{y}_{obs} | \mathbf{x}, \theta, \hat{\beta}(\mathbf{d}), \hat{\beta}_d(\mathbf{d}), \hat{\beta}_e(\mathbf{d}), \epsilon_{obs}^*)$ is the likelihood function and q_i is the i -th calibration parameter. Note that $\theta, \hat{\beta}(\mathbf{d}), \hat{\beta}_d(\mathbf{d}), \hat{\beta}_e(\mathbf{d})$ is used in $L(\mathbf{y}_{obs}, \mathbf{x}) = L(\mathbf{y}_{obs} | \mathbf{x}, \theta, \hat{\beta}(\mathbf{d}), \hat{\beta}_d(\mathbf{d}), \hat{\beta}_e(\mathbf{d}), \epsilon_{obs}^*)$ instead of $\theta^*, \hat{\beta}^*(\mathbf{d}^*), \hat{\beta}_d^*(\mathbf{d}^*), \hat{\beta}_e^*(\mathbf{d}^*)$ because $\theta, \hat{\beta}(\mathbf{d}), \hat{\beta}_d(\mathbf{d}), \hat{\beta}_e(\mathbf{d})$ are dependent on θ . Details about the proof and derivation of Eq. (36) are available in Refs. [7, 18].

Suppose that n_{obs} observations of the field response are collected, Eq. (36) is written as

$$\hat{I}_{ij}(\mathbf{y}_{obs}) = - \sum_{k=1}^{n_{obs}} \frac{1}{q_i q_j} \log(L(\mathbf{y}_{obs}^{[k]}, \mathbf{x}^{[k]})) \quad (37)$$

$$\mathbf{\theta} = \mathbf{\theta}^*, \hat{\boldsymbol{\beta}}(\mathbf{d}) = \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d(\mathbf{d}) = \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e(\mathbf{d}) = \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*)$$

$$, \quad i, j = 1, 2, L, n_q,$$

where $L(\mathbf{y}_{obs}^{[k]}, \mathbf{x}^{[k]}) = L(\mathbf{y}_{obs}^{[k]} | \mathbf{x}^{[k]}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^{[k]})$, in which $\mathbf{x}^{[k]}$ and $\boldsymbol{\varepsilon}_{obs}^{[k]}$ are the input setting and observation errors of the k -th observation and $\mathbf{y}_{obs}^{[k]}$ is corresponding field observation.

Since $\hat{I}_{ij}(\mathbf{y}_{obs})$ of multiple observation case is just a summation of that of individual observation, in the subsequent section, we use the one observation case (one observation of field response) to illustrate how to solve Eq. (36). As shown in Fig. 2, for given $\mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d})$, and $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$, $L(\mathbf{y}_{obs} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^*)$ is computed by

$$L(\mathbf{y}_{obs} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^*) = \frac{1}{\sqrt{(2\pi)^{n_z} |\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\mathbf{y}_{obs} - \hat{\boldsymbol{\mu}}_{Obs})^T \boldsymbol{\Sigma}^{-1}(\mathbf{y}_{obs} - \hat{\boldsymbol{\mu}}_{Obs})\right\} \quad (38)$$

where $\boldsymbol{\Sigma}^{-1}$ is a covariance matrix which is only related to observation error (independent from $\mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d})$, and $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$) and $\hat{\boldsymbol{\mu}}_{Obs} = \hat{\boldsymbol{\mu}}_{Y_{obs}} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d})$, which is given by

$$\hat{\boldsymbol{\mu}}_{Y_{obs}} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}) = \sum_{k=1}^r \hat{b}_k(\mathbf{d}) j_k(\mathbf{z}) + \sum_{k=1}^{r_e} \hat{b}_{e,k}(\mathbf{d}) j_{e,k}(\mathbf{z}) + \sum_{k=1}^{r_d} \hat{b}_{dk}(\mathbf{d}) j_{dk}(\mathbf{z}), \quad (39)$$

$$\mathbf{z} = \mathbf{W}_Z \mathbf{x} + \mathbf{W}_u \mathbf{x}_u,$$

and $\mathbf{y}_{obs} = (\hat{\boldsymbol{\mu}}_{Y_{obs}} | \mathbf{x}, \mathbf{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*)) + \boldsymbol{\varepsilon}_{obs}^*$. Note that the mean value expression given in Eq. (39) is different from that given in Eq. (31) because Eq. (39) is the mean of conditional likelihood $L(\mathbf{y}_{obs} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^*)$. After substituting Eq. (38) into Eq. (36), we have

$$\begin{aligned} & \frac{1}{q_i q_j} \log(L(\mathbf{y}_{obs} | \mathbf{x}, \mathbf{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^*)) \\ &= \frac{1}{q_i q_j} \boldsymbol{\mu}_{Obs}^T \boldsymbol{\Sigma}^{-1}(\mathbf{y}_{obs} - \boldsymbol{\mu}_{Obs}) - \frac{1}{q_i} \boldsymbol{\mu}_{Obs}^T \boldsymbol{\Sigma}^{-1} \frac{1}{q_j} \boldsymbol{\mu}_{Obs}, \end{aligned} \quad (40)$$

where
$$\frac{\mathbb{P}(\mathbf{m}_{Obs})}{\mathbb{P}(q_j)} = \frac{\mathbb{P}(m_{Obs}(\mathbf{z}^{(1)}))}{\mathbb{P}(q_j)}, \frac{\mathbb{P}(m_{Obs}(\mathbf{z}^{(2)}))}{\mathbb{P}(q_j)}, \dots, \frac{\mathbb{P}(m_{Obs}(\mathbf{z}^{(n_Z)}))}{\mathbb{P}(q_j)} \quad i = 1 \dots n_Z$$
 and

$$m_{Obs}(\mathbf{z}^{(i)}) = m_{Obs}(\mathbf{z}^{(i)}) \Big| \mathbf{x}, \boldsymbol{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), i = 1, 2, \dots, n_Z.$$

Eq. (40) shows that the Jacobian and Hessian matrices of $\hat{\boldsymbol{\mu}}_{Obs}$ are critical elements for solving Eq. (36). Since $\hat{\boldsymbol{\beta}}(\mathbf{d}) = [\hat{b}_1(\mathbf{d}), \dots, \hat{b}_r(\mathbf{d})]$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d}) = [\hat{b}_{d,1}(\mathbf{d}), \dots, \hat{b}_{d,r_d}(\mathbf{d})]$, and $\hat{\boldsymbol{\beta}}_e(\mathbf{d}) = [\hat{b}_{e,1}(\mathbf{d}), \dots, \hat{b}_{e,r_e}(\mathbf{d})]$ are random variables conditioned on $\boldsymbol{\theta}$, this causes difficulty in computing the derivatives. In order to overcome this difficulty, we first transform $\boldsymbol{\theta}$, $\hat{\boldsymbol{\beta}}(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_d(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$, and $\boldsymbol{\varepsilon}_{Obs}$ into standard normal random variables by using the Rosenblatt transformation [39] as below:

$$\begin{aligned} \mathbf{U}_{\boldsymbol{\theta}} &= \Phi^{-1}(F_{\boldsymbol{\theta}}(\boldsymbol{\theta})), \\ \mathbf{U}_{\boldsymbol{\varepsilon}_{Obs}} &= \Phi^{-1}(F_{\boldsymbol{\varepsilon}_{Obs}}(\boldsymbol{\varepsilon}_{Obs})), \\ \mathbf{U}_{\hat{\boldsymbol{\beta}}(\mathbf{d})} &= \Phi^{-1}(F_{\hat{\boldsymbol{\beta}}(\mathbf{d})}(\hat{\boldsymbol{\beta}}(\mathbf{d}))), \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})} = \Phi^{-1}(F_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}(\hat{\boldsymbol{\beta}}_d(\mathbf{d}))), \mathbf{U}_{\hat{\boldsymbol{\beta}}_e(\mathbf{d})} = \Phi^{-1}(F_{\hat{\boldsymbol{\beta}}_e(\mathbf{d})}(\hat{\boldsymbol{\beta}}_e(\mathbf{d}))), \end{aligned} \quad (41)$$

where $\Phi^{-1}(\cdot)$ is the inverse cumulative density function (CDF) of a standard normal variable, $F_X(x)$ is the CDF of a random variable X , and U_X is the standard normal variable corresponding to random variable X . Note that the Rosenblatt transformation is used here because $\hat{\boldsymbol{\beta}}(\mathbf{d})$, $\hat{\boldsymbol{\beta}}_e(\mathbf{d})$, and $\hat{\boldsymbol{\beta}}_d(\mathbf{d})$ are conditioned on $\boldsymbol{\theta}$.

After the Rosenblatt transformation, the CEDO model given in Eq. (34) is rewritten as

$$\begin{aligned} \min_{\mathbf{x}} F(\mathbf{x}) &= \{w_1 S_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{Obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{Obs}, \mathbf{x})) \\ &\quad - w_2 E_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{Obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{Obs}, \mathbf{x}))\}, \\ \text{s.t. } \mathbf{x} &\in [\mathbf{x}_l, \mathbf{x}_u]. \end{aligned} \quad (42)$$

Eq. (36) is rewritten as

$$\hat{I}_{ij}(\mathbf{y}_{obs}) = - \frac{\sum_{i=1}^L \sum_{j=1}^{n_q} \mathbb{I}_{q_i}^2}{\sum_{i=1}^L \sum_{j=1}^{n_q} \mathbb{I}_{q_i} \mathbb{I}_{q_j}} \log(L(\mathbf{y}_{obs}, \mathbf{x})) \Big|_{\mathbf{U}_0 = \mathbf{u}_0, \mathbf{U}_{\hat{\beta}} = \mathbf{u}_{\hat{\beta}}, \mathbf{U}_{\hat{\beta}_e} = \mathbf{u}_{\hat{\beta}_e}, \mathbf{U}_{\hat{\beta}_d(\mathbf{d})} = \mathbf{u}_{\hat{\beta}_d(\mathbf{d})}}, i, j = 1, 2, L, n_q, \quad (43)$$

where $L(\mathbf{y}_{obs}, \mathbf{x}) = L(\mathbf{y}_{obs} | \mathbf{x}, \mathbf{U}_0, \mathbf{U}_{\hat{\beta}}, \mathbf{U}_{\hat{\beta}_d}, \mathbf{U}_{\hat{\beta}_e}(\mathbf{d}), \mathbf{u}_{e_{obs}})$, $\mathbf{u}_0 = \Phi^{-1}(F_{\theta}(\theta^*))$, $\mathbf{u}_{e_{obs}} = \Phi^{-1}(F_{e_{obs}}(\epsilon_{obs}^*))$, and $\mathbf{u}_{\hat{\beta}}, \mathbf{u}_{\hat{\beta}_d}, \mathbf{u}_{\hat{\beta}_e}$ are associated with $\hat{\beta}^*(\mathbf{d}^*), \hat{\beta}_d^*(\mathbf{d}^*), \hat{\beta}_e^*(\mathbf{d}^*)$ similarly.

In the above equations, $\mathbf{U}_{\hat{\beta}}, \mathbf{U}_{\hat{\beta}_d}, \mathbf{U}_{\hat{\beta}_e}, \mathbf{U}_0, \mathbf{U}_{e_{obs}}$ are independent standard normal variables.

Since the predictions from the Kriging surrogate model follow a normal distribution, we have

$$\hat{\beta}(\mathbf{d}) = \mu_{\beta}(\mathbf{d}) + \mathbf{U}_{\hat{\beta}(\mathbf{d})} \sigma_{\beta}(\mathbf{d})^T. \quad (44)$$

The above equation is also applicable to $\hat{\beta}_e(\mathbf{d})$ and $\hat{\beta}_d(\mathbf{d})$. Substituting Eq. (44) into Eq. (39), we have

$$\begin{aligned} \hat{\mu}_{Y_{obs}} | \mathbf{x}, \theta, \hat{\beta}(\mathbf{d}), \hat{\beta}_d(\mathbf{d}), \hat{\beta}_e(\mathbf{d}) &= \hat{\mu}_{Y_{obs}} | \mathbf{x}, \mathbf{U}_0, \mathbf{U}_{\hat{\beta}}, \mathbf{U}_{\hat{\beta}_d}, \mathbf{U}_{\hat{\beta}_e} = \sum_{k=1}^r (m_{\hat{\beta}_k}(\mathbf{d}) + U_{\hat{\beta}_k} s_{\hat{\beta}_k}(\mathbf{d})) j_k(\mathbf{z}) \\ &+ \sum_{k=1}^{r_e} (m_{\hat{\beta}_{e,k}}(\mathbf{d}) + U_{\hat{\beta}_{e,k}} s_{\hat{\beta}_{e,k}}(\mathbf{d})) j_{e,k}(\mathbf{z}) + \sum_{k=1}^{r_d} (m_{\hat{\beta}_{d,k}}(\mathbf{d}) + U_{\hat{\beta}_{d,k}} s_{\hat{\beta}_{d,k}}(\mathbf{d})) j_{d,k}(\mathbf{z}), \end{aligned} \quad (45)$$

" $\mathbf{z} \hat{W}_Z, \mathbf{x} \hat{W}_Z, \mathbf{x} \hat{W}_Z$], and $\theta \hat{W}_0$.

With Eq. (45), we can then compute the Jacobian and Hessian matrices of $\hat{\mu}_{obs}$ as follows:

$$\begin{aligned} \frac{\mathbb{I} \hat{\mu}_{obs}}{\mathbb{I} q_i} &= \sum_{k=1}^r \left(\frac{\mathbb{I} m_{\hat{\beta}_k}(\mathbf{d})}{\mathbb{I} q_i} + U_{\hat{\beta}_k} \frac{\mathbb{I} s_{\hat{\beta}_k}(\mathbf{d})}{\mathbb{I} q_i} \right) j_k(\mathbf{z}) + \sum_{k=1}^{r_e} \left(\frac{\mathbb{I} m_{\hat{\beta}_{e,k}}(\mathbf{d})}{\mathbb{I} q_i} + U_{\hat{\beta}_{e,k}} \frac{\mathbb{I} s_{\hat{\beta}_{e,k}}(\mathbf{d})}{\mathbb{I} q_i} \right) j_{e,k}(\mathbf{z}) \\ &+ \sum_{k=1}^{r_d} \left(\frac{\mathbb{I} m_{\hat{\beta}_{d,k}}(\mathbf{d})}{\mathbb{I} q_i} + U_{\hat{\beta}_{d,k}} \frac{\mathbb{I} s_{\hat{\beta}_{d,k}}(\mathbf{d})}{\mathbb{I} q_i} \right) j_{d,k}(\mathbf{z}), \quad "i = 1, 2, \dots, n_q, \mathbf{z} \hat{W}_Z, \mathbf{x} \hat{W}_Z, \mathbf{x} \hat{W}_Z, \text{ and } \theta \hat{W}_0, \end{aligned} \quad (46)$$

and

$$\begin{aligned} \frac{\mathbb{I}^2 \hat{\mu}_{obs}^T}{\mathbb{I} q_i \mathbb{I} q_j} &= \sum_{k=1}^r \left(\frac{\mathbb{I}^2 m_{\hat{\beta}_k}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} + U_{\hat{\beta}_k} \frac{\mathbb{I}^2 s_{\hat{\beta}_k}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} \right) j_k(\mathbf{z}) + \sum_{k=1}^{r_e} \left(\frac{\mathbb{I}^2 m_{\hat{\beta}_{e,k}}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} + U_{\hat{\beta}_{e,k}} \frac{\mathbb{I}^2 s_{\hat{\beta}_{e,k}}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} \right) j_{e,k}(\mathbf{z}) \\ &+ \sum_{k=1}^{r_d} \left(\frac{\mathbb{I}^2 m_{\hat{\beta}_{d,k}}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} + U_{\hat{\beta}_{d,k}} \frac{\mathbb{I}^2 s_{\hat{\beta}_{d,k}}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} \right) j_{d,k}(\mathbf{z}), \quad "i, j = 1, 2, \dots, n_q, \mathbf{z} \hat{W}_Z, \mathbf{x} \hat{W}_Z, \mathbf{x} \hat{W}_Z, \text{ and } \theta \hat{W}_0. \end{aligned} \quad (47)$$

Since $\boldsymbol{\mu}_b(\mathbf{d}) = [m_{b_1}(\mathbf{d}), m_{b_2}(\mathbf{d}), \dots, m_{b_r}(\mathbf{d})]$, and $s_{b_k}^2(\mathbf{d})$, $k = 1, 2, \dots, r$, are predicted from Kriging surrogate models, we can compute their derivatives based on the Kriging surrogate model predictions. Based on Eqs. (A4) and (A6) given in the Appendix, $\frac{\mathbb{I} m_{b_k}(\mathbf{d})}{\mathbb{I} q_i}$, $\frac{\mathbb{I} s_{b_k}^2(\mathbf{d})}{\mathbb{I} q_i}$,

$\frac{\mathbb{I}^2 m_{b_k}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j}$, and $\frac{\mathbb{I}^2 s_{b_k}^2(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j}$ are derived as

$$\frac{\mathbb{I} m_{b_k}(\mathbf{d})}{\mathbb{I} q_i} = \frac{\mathbb{I} \mathbf{h}(\mathbf{d})^T}{\mathbb{I} q_i} \mathbf{v} + \frac{\mathbb{I} \mathbf{r}(\mathbf{d})^T}{\mathbb{I} q_i} \mathbf{R}^{-1}(\mathbf{g} - \mathbf{H}\mathbf{v}), \quad (48)$$

$$\begin{aligned} \frac{\mathbb{I} s_{b_k}^2(\mathbf{d})}{\mathbb{I} q_i} &= 2s_e^2 \left\{ -\frac{\mathbf{r}(\mathbf{d})^T \mathbf{R}^{-1} \mathbb{I} \mathbf{r}(\mathbf{d})}{\mathbb{I} q_i} \right. \\ &\quad \left. + [\mathbf{H}^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{d}) - \mathbf{h}(\mathbf{d})]^T (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} [\mathbf{H}^T \mathbf{R}^{-1} \frac{\mathbb{I} \mathbf{r}(\mathbf{d})}{\mathbb{I} q_i} - \frac{\mathbb{I} \mathbf{h}(\mathbf{d})}{\mathbb{I} q_i}] \right\}, \end{aligned} \quad (49)$$

$$\frac{\mathbb{I}^2 m_{b_k}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} = \frac{\mathbb{I}^2 \mathbf{h}(\mathbf{d})^T}{\mathbb{I} q_i \mathbb{I} q_j} \mathbf{v} + \frac{\mathbb{I}^2 \mathbf{r}(\mathbf{d})^T}{\mathbb{I} q_i \mathbb{I} q_j} \mathbf{R}^{-1}(\mathbf{g} - \mathbf{H}\mathbf{v}), \quad (50)$$

$$\begin{aligned} \frac{\mathbb{I}^2 s_{b_k}^2(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} &= 2s_e^2 \left\{ -\frac{\mathbb{I} \mathbf{r}(\mathbf{d})^T}{\mathbb{I} q_i} \mathbf{R}^{-1} \frac{\mathbb{I} \mathbf{r}(\mathbf{d})}{\mathbb{I} q_j} - \frac{\mathbf{r}(\mathbf{d})^T \mathbf{R}^{-1} \mathbb{I}^2 \mathbf{r}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} \right. \\ &\quad \left. + [\mathbf{H}^T \mathbf{R}^{-1} \frac{\mathbb{I} \mathbf{r}(\mathbf{d})}{\mathbb{I} q_i} - \frac{\mathbb{I} \mathbf{h}(\mathbf{d})}{\mathbb{I} q_i}]^T (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} [\mathbf{H}^T \mathbf{R}^{-1} \frac{\mathbb{I} \mathbf{r}(\mathbf{d})}{\mathbb{I} q_j} - \frac{\mathbb{I} \mathbf{h}(\mathbf{d})}{\mathbb{I} q_j}] \right. \\ &\quad \left. + [\mathbf{H}^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{d}) - \mathbf{h}(\mathbf{d})]^T (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} [\mathbf{H}^T \mathbf{R}^{-1} \frac{\mathbb{I}^2 \mathbf{r}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j} - \frac{\mathbb{I}^2 \mathbf{h}(\mathbf{d})}{\mathbb{I} q_i \mathbb{I} q_j}] \right\}, \end{aligned} \quad (51)$$

where $\mathbf{v}$, $\mathbf{H}$, $\mathbf{R}$, and $\mathbf{g}$ are given in Eq. (A3) in the Appendix.

When a constant trend function is used in the Kriging model, we have $\mathbb{I} \mathbf{h}(\mathbf{d})^T / \mathbb{I} q_i = \mathbf{0}$ and the above equations can be simplified. It implies that the basics of computing the derivatives is to solve the derivatives of the correlation functions (i.e. exponential, Gaussian, and etc.) in the Kriging models. Since the function formats of these correlation functions are explicitly known,

the derivatives can also be computed analytically. For example, for the widely used Gaussian correlation function, we have

$$\frac{\partial^2 \mathbf{r}(\mathbf{d})}{\partial \theta_i \partial \theta_j} = 4l_i l_j [R(\mathbf{d}, \mathbf{d}_1) \Delta \theta_i^{(1)} \Delta \theta_j^{(1)}, R(\mathbf{d}, \mathbf{d}_2) \Delta \theta_i^{(2)} \Delta \theta_j^{(2)}, \dots, R(\mathbf{d}, \mathbf{d}_{n_s}) \Delta \theta_i^{(n_s)} \Delta \theta_j^{(n_s)}], \quad i \neq j, \quad (52)$$

where $R(\mathbf{d}, \mathbf{d}_k)$ is given in Eq. (A2), l_i and l_j are the correlation parameters of θ_i and θ_j and $\Delta \theta_i^{(k)}$ is the distance between current θ_i and θ_i of the k -th training point.

With the Jacobian and Hessian matrices of $s_{b_k}^2(\mathbf{d})$, the Jacobian and Hessian matrices of $s_{\hat{b}_k}(\mathbf{d})$ is computed by

$$\frac{\mathbb{J} s_{\hat{b}_k}(\mathbf{d})}{\mathbb{J} q_i} = \frac{1}{2s_{b_k}^2(\mathbf{d})} \frac{\mathbb{J} s_{b_k}^2(\mathbf{d})}{\mathbb{J} q_i}, \quad (53)$$

and

$$\frac{\mathbb{J}^2 s_{\hat{b}_k}(\mathbf{d})}{\mathbb{J} q_i \mathbb{J} q_j} = \frac{-1}{2s_{b_k}^2(\mathbf{d})} \frac{\mathbb{J} s_{\hat{b}_k}(\mathbf{d})}{\mathbb{J} q_j} \frac{\mathbb{J} s_{b_k}^2(\mathbf{d})}{\mathbb{J} q_i} + \frac{1}{2s_{b_k}^2(\mathbf{d})} \frac{\mathbb{J}^2 s_{b_k}^2(\mathbf{d})}{\mathbb{J} q_i \mathbb{J} q_j}, \quad (54)$$

in which $s_{b_k}^2(\mathbf{d})$ is given in Eq. (A6).

The Jacobian and Hessian matrices of $\mu_{b_d}(\mathbf{d})$, $\mu_{b_e}(\mathbf{d})$, $\sigma_{b_d}(\mathbf{d})$, and $\sigma_{b_e}(\mathbf{d})$ are computed similarly using the above equations. With Eqs. (45) through (54), Eq. (43) (i.e. Eq. (36)) can be solved analytically.

Since $\mathbf{y}_{obs}$ is computed using Eq. (33), when the observation errors are assumed to follow independent normal distributions, Eq. (40) is simplified as follows

$$\frac{\mathbb{J}^2 \log(L(\mathbf{y}_{obs} | \mathbf{x}, \boldsymbol{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}^*))}{\mathbb{J} q_i \mathbb{J} q_j} = \frac{\mathbb{J}^2 \hat{\boldsymbol{\mu}}_{Obs}^T \boldsymbol{\Sigma}^{-1} \mathbf{U}_{e_{obs}} s_{e_{obs}}}{\mathbb{J} q_i \mathbb{J} q_j} - \frac{\mathbb{J} \hat{\boldsymbol{\mu}}_{Obs}^T \boldsymbol{\Sigma}^{-1} \mathbb{J} \hat{\boldsymbol{\mu}}_{Obs}}{\mathbb{J} q_i \mathbb{J} q_j}. \quad (55)$$

where $\hat{\boldsymbol{\mu}}_{Obs} = \hat{\boldsymbol{\mu}}_{Y_{obs}} | \mathbf{x}, \boldsymbol{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}) = \hat{\boldsymbol{\mu}}_{Y_{obs}} | \mathbf{x}, \mathbf{U}_0, \mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}$.

Based on the above equations, Eq. (43) (i.e. Eq. (36)) can be solved analytically and the posterior distribution $\pi_{post}(\boldsymbol{\theta}|\mathbf{y}_{obs}, \mathbf{x}, \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), e_{obs}^*)$ given in Eq. (35) is estimated.

The expressions given in Eqs. (48) and (50) show that the Jacobian and Hessian of the mean value predictions are required to compute the Fisher information matrix. For some problems, the Jacobian and Hessian can be efficiently computed using the adjoint method and automatic differentiation tools [40], such as in computational fluid dynamics (CFD) simulation problems. In that situation, building surrogate models directly for the Jacobian and Hessian and using the gradient information to improve the accuracy of the response surrogate model can significantly improve the accuracy of experimental design. Using the adjoint method to improve the accuracy of CEDO will be investigated in our future work.

(b) *Estimation of $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})|\boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\epsilon}_{obs}^*$ (K-L divergence)*

Based on the multivariate normal distribution approximation of the posterior distribution given in Eq. (35), an analytical estimation of the K-L divergence $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})$ has been derived in Ref. [7] based on Taylor series expansion as

$$D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) \gg -\frac{1}{2}\log((2p)^{n_q} |\hat{\mathbf{I}}(\mathbf{y}_{obs})^{-1}|) - \frac{n_q}{2} - h(\boldsymbol{\theta}) - \frac{tr(\hat{\mathbf{I}}(\mathbf{y}_{obs})^{-1} \tilde{\mathbf{N}} \tilde{\mathbf{N}} h(\boldsymbol{\theta}))}{2}, \quad (56)$$

where $h(\boldsymbol{\theta}) = \log(\pi_0(\boldsymbol{\theta}))$. Detailed derivations are available in Ref. [7].

In this paper the above equation is used to estimate $D_{KL}(\mathbf{y}_{obs}, \mathbf{x})$. If non-informative uniform distributions are used as priors, then we have

$$D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) \gg -\frac{1}{2}\log((2p)^{n_q} |\hat{\mathbf{I}}(\mathbf{y}_{obs})^{-1}|) - \frac{n_q}{2} + \log(D\boldsymbol{\theta}), \quad (57)$$

where $D\boldsymbol{\theta}$ is the product of the width of the uniform distributions.

3.4.2. Estimation of the objective function

Even though there is an analytical approximation of $D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) | \boldsymbol{\theta}^*, \hat{\boldsymbol{\beta}}^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_d^*(\mathbf{d}^*), \hat{\boldsymbol{\beta}}_e^*(\mathbf{d}^*), \boldsymbol{\varepsilon}_{obs}^*$, solving the $E_{\hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ and $s_{\hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d}), \boldsymbol{\varepsilon}_{obs}, \boldsymbol{\theta}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ is still computationally very expensive due to the required high-dimensional integrations. As shown in Eq. (42), $\boldsymbol{\theta}, \hat{\boldsymbol{\beta}}(\mathbf{d}), \hat{\boldsymbol{\beta}}_d(\mathbf{d}), \hat{\boldsymbol{\beta}}_e(\mathbf{d})$, and $\boldsymbol{\varepsilon}_{obs}$ have been transformed into independent standard normal variables $\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d}, \mathbf{U}_{\boldsymbol{\theta}}$, and $\mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}$. The task now is how to solve $E_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ and $s_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$. When the dimension of $\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}$ is low, the objective function of Eq. (42) is directly solved using the numerical integration method. When the dimension of $\boldsymbol{\theta}$ is high, in this paper, the objective function of Eq. (42) is solved using the Monte Carlo simulation (MCS) as follows [41]

$$E(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) \approx \frac{1}{N_{MCS}} \sum_{i=1}^{N_{MCS}} D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) | \mathbf{u}_{\hat{\boldsymbol{\beta}}}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_e}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_d}^{(i)}, \mathbf{u}_{\boldsymbol{\theta}}^{(i)}, \mathbf{u}_{\boldsymbol{\varepsilon}_{obs}}^{(i)}, \quad (58)$$

and

$$s^2(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) \approx \frac{1}{N_{MCS} - 1} \sum_{i=1}^{N_{MCS}} (D_{KL}(\mathbf{y}_{obs}, \mathbf{x}) | \mathbf{u}_{\hat{\boldsymbol{\beta}}}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_e}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_d}^{(i)}, \mathbf{u}_{\boldsymbol{\theta}}^{(i)}, \mathbf{u}_{\boldsymbol{\varepsilon}_{obs}}^{(i)} - E(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})))^2, \quad (59)$$

where

$$E(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) = E_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})),$$

$s^2(D_{KL}(\mathbf{y}_{obs}, \mathbf{x})) = s_{\mathbf{U}_{\hat{\boldsymbol{\beta}}}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_e}, \mathbf{U}_{\hat{\boldsymbol{\beta}}_d(\mathbf{d})}, \mathbf{U}_{\boldsymbol{\theta}}, \mathbf{U}_{\boldsymbol{\varepsilon}_{obs}}, \mathbf{x}}(D_{KL}(\mathbf{y}_{obs}, \mathbf{x}))$ for the sake of illustration, N_{MCS} is the total number of MCS samples and $\mathbf{u}_{\hat{\boldsymbol{\beta}}}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_e}^{(i)}, \mathbf{u}_{\hat{\boldsymbol{\beta}}_d}^{(i)}, \mathbf{u}_{\boldsymbol{\theta}}^{(i)}, \mathbf{u}_{\boldsymbol{\varepsilon}_{obs}}^{(i)}$ is the i -th MCS sample.

There may have uncertainty in the above MCS estimations due to the limited number of samples. The variances of the above estimations can be estimated [41] based on the results of Eqs. (58) and (59). Since N_{MCS} is selected as a large number in this paper, we assume that the MCS estimate is accurate. Besides, in order to achieve a quick converge, the Latin Hypercube Sample (LHS) method [42] is employed in this paper to generate MCS samples.

3.5. Solution of the CEDO model

Since surrogate models are used in the CEDO model, we first propose a global sensitivity analysis (GSA)-based method to check the quality of the surrogate models. After that, we discuss how to solve the CEDO model.

3.5.1. Global sensitivity analysis (GSA) for quality check of surrogate models

If there are no surrogate models involved in CEDO, for a given value of $\mathbf{x}$ and $\boldsymbol{\theta}$, the objective function $F(\mathbf{x})|\boldsymbol{\theta}, \mathbf{x}$ in Eq. (11) is a deterministic value since we only have uncertainty in $\mathbf{U}_{e_{obs}}$. If the epistemic uncertainty in $\boldsymbol{\theta}$ is also considered in a Bayesian framework, $F(\mathbf{x})|\boldsymbol{\theta}, \mathbf{x}$ is uncertain due to the lack of knowledge in $\boldsymbol{\theta}$. The uncertainty of $F(\mathbf{x})|\boldsymbol{\theta}, \mathbf{x}$ then comes from the uncertainty of $\mathbf{U}_\theta$ (the standard normal variables transformed from $\boldsymbol{\theta}$ in Eq. (41)). Or in other words, the contribution of $\mathbf{U}_\theta$ to the uncertainty of $F(\mathbf{x})|\boldsymbol{\theta}, \mathbf{x}$ is one.

After using surrogate models to substitute for the original simulation model, model discrepancy, and discretization error, extra uncertainty sources are introduced, which include $\mathbf{U}_{\hat{b}}$, $\mathbf{U}_{\hat{b}_e}$, and $\mathbf{U}_{\hat{b}_d}$. The contribution of $\mathbf{U}_\theta$ to the uncertainty of $F(\mathbf{x})|\boldsymbol{\theta}, \mathbf{x}$ is then less than one. $\mathbf{U}_\theta$, $\mathbf{U}_{\hat{b}}$, $\mathbf{U}_{\hat{b}_e}$, and $\mathbf{U}_{\hat{b}_d}$ are all epistemic uncertainty which are reducible. However, the epistemic

uncertainty of $\mathbf{U}_{\hat{b}_d}$ and $\mathbf{U}_\theta$ can only be reduced by tests, which have not been performed yet during CEDO. On the other hand, the epistemic uncertainty of $\mathbf{U}_{\hat{b}}$ and $\mathbf{U}_{\hat{b}_e}$ can be reduced by performing more simulations and adding more training points to the surrogate models. Based on this, we classify various sources of model uncertainty into two groups: *reducible during CEDO* ($\mathbf{U}_{\hat{b}}$ and $\mathbf{U}_{\hat{b}_e}$) and *irreducible during CEDO* ($\mathbf{U}_{\hat{b}_d}$ and $\mathbf{U}_\theta$).

Since the epistemic uncertainty in $\mathbf{U}_{\hat{b}}$ and $\mathbf{U}_{\hat{b}_e}$ can be reduced without testing, we investigate their effects on CEDO. In this paper, we propose to check the quality of the surrogate models (i.e. $\mathbf{U}_{\hat{b}}$ and $\mathbf{U}_{\hat{b}_e}$) by analyzing their contributions to the uncertainty of the objective function. If the contribution of the reducible uncertainty sources is smaller than a desired threshold, the surrogate models are ready to be used for CEDO. Otherwise, we adaptively add more training points in the regions where the contribution is high to first improve the quality of the surrogate model before proceeding to CEDO.

In this paper, the Sobol indices-based global sensitivity analysis (GSA) [43] is employed to perform uncertainty contribution analysis. For a given design variable $\mathbf{x}$, $\mathbf{U}_{\hat{b}} = \mathbf{u}_{\hat{b}}$, $\mathbf{U}_{\hat{b}_e} = \mathbf{u}_{\hat{b}_e}$, $\mathbf{U}_{\hat{b}_d} = \mathbf{u}_{\hat{b}_d}$, and $\mathbf{U}_\theta = \mathbf{u}_\theta$, $F(\mathbf{x})|_{\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_\theta}$ is computed by

$$F(\mathbf{x})|_{\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_\theta} = w_1 \frac{\sum_{i=1}^{N_{MCS}} (D_{KL}(\mathbf{y}_{obs}, \mathbf{x})|_{\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_\theta, \mathbf{u}_{e_{obs}}^{(i)} - m_{D_{KL}}|_{\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_\theta})^2}{N_{MCS} - 1} + w_2 \frac{1}{N_{MCS}} \sum_{i=1}^{N_{MCS}} D_{KL}(\mathbf{y}_{obs}, \mathbf{x})|_{\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_\theta, \mathbf{u}_{e_{obs}}^{(i)}} \quad (60)$$

Defining $\mathbf{U}_{model} = [\mathbf{U}_{\hat{b}}, \mathbf{U}_{\hat{b}_e}, \mathbf{U}_{\hat{b}_d}, \mathbf{U}_\theta]$ and $\mathbf{U}_{g1} = [\mathbf{U}_{\hat{b}}, \mathbf{U}_{\hat{b}_e}]$, the first order index of $\mathbf{U}_{g1}$ is then computed by

$$S_{\mathbf{U}_{g1}}^1(\mathbf{x}) = V_{\mathbf{U}_{\hat{b}}} (E_{\mathbf{U}_{\text{model-g1}}} (F(\mathbf{x})|\mathbf{u}_{g1})) / V_{\mathbf{U}_{\text{model}}} (F(\mathbf{x})), \quad (61)$$

where $\mathbf{U}_{\text{model-g1}}$ are all the other random variables in $\mathbf{U}_{\text{model}}$ excluding $\mathbf{U}_{g1}$, $E_{\mathbf{U}_{\text{model-g1}}} (F(\mathbf{x})|\mathbf{u}_{g1})$ is the expectation of Eq. (60) by fixing $\mathbf{U}_{g1}$ at $\mathbf{u}_{g1}$, and $V_{\mathbf{U}_{\text{model}}} (F(\mathbf{x}))$ is the variance of Eq. (60) by considering all uncertainty variables in $\mathbf{U}_{\text{model}}$.

There are three loops of computation in Eq. (61). The first loop is the estimation of Eq. (60). The second loop computes $E_{\mathbf{U}_{\text{model-b}}} (\otimes)$, and the third loop computes $V_{\mathbf{U}_{\hat{b}}} (\otimes)$. Since Eq. (60) considers only the observation error, which is usually very small, an analytical expression of Eq. (60) can be obtained using first-order Taylor series expansion. We expand $F(\mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}$ at the mean values of $\mathbf{U}_{e_{\text{obs}}}$. After expansion, $F(\mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}$ is computed by

$$F(\mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta} = w_1 \left\| \frac{\mathbf{q} D_{KL}(\mathbf{y}_{\text{obs}}, \mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}, \mathbf{U}_{e_{\text{obs}}}}{\mathbf{q} \mathbf{U}_{e_{\text{obs}}}} \right\|_{\mathbf{U}_{e_{\text{obs}}} = \mathbf{0}} \quad (62)$$

$$- w_2 (D_{KL}(\mathbf{y}_{\text{obs}}, \mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}, \mathbf{0}),$$

where $\|\cdot\|$ is the norm of a vector and the component of the derivative vector is derived as

$$\frac{\mathbf{q} D_{KL}(\mathbf{y}_{\text{obs}}, \mathbf{x})|\mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}, \mathbf{U}_{e_{\text{obs}}}}{\mathbf{q} \mathbf{U}_{e_{\text{obs}}}} = 0.5 \text{tr} \left(\frac{\mathbf{q} \hat{\mathbf{I}}(\mathbf{y}_{\text{obs}})}{\mathbf{q} \mathbf{U}_{e_{\text{obs}}}} \hat{\mathbf{I}}(\mathbf{y}_{\text{obs}})^{-1} \right) \quad (63)$$

in which $\mathbf{q} \hat{\mathbf{I}}(\mathbf{y}_{\text{obs}}) / \mathbf{q} \mathbf{U}_{e_{\text{obs}}}$ can be obtained analytically using the method discussed in Sec. 3.4.1

and $\text{tr}(\otimes)$ is the trace of a matrix.

For instance, the (i, j) -th element of $\mathbf{q} \hat{\mathbf{I}}(\mathbf{y}_{\text{obs}}) / \mathbf{q} \mathbf{U}_{e_{\text{obs}}}$ is given by

$$\frac{\mathbf{q} \hat{I}_{ij}(\mathbf{y}_{\text{obs}})}{\mathbf{q} \mathbf{U}_{e_{\text{obs}}}} = - \frac{\mathbf{q}}{\mathbf{q} \mathbf{U}_{e_{\text{obs}}}} \frac{\dot{\mathbf{q}}^2}{\mathbf{q} q_i q_j} \log(L(\mathbf{y}_{\text{obs}}|\mathbf{\theta}, \mathbf{x})) \Big|_{\mathbf{\theta}=\mathbf{\hat{\theta}}} \quad (64)$$

where

$$\frac{\prod_{e_{obs}} \frac{\hat{\epsilon}}{\epsilon} \prod_j^2}{\prod_i q_i \prod_j q_j} \log(L(\mathbf{y}_{obs} | \boldsymbol{\theta}, \mathbf{x})) = \frac{\prod_i^2 \hat{\boldsymbol{\mu}}_{y_{obs}}^T}{\prod_i q_i \prod_j q_j} \boldsymbol{\Sigma}^{-1} \mathbf{s}_{e_{obs}}. \quad (65)$$

The above equation is obtained using Eq. (55). Based on Eqs. (62) through (65), $F(\mathbf{x}) | \mathbf{u}_{\hat{b}}, \mathbf{u}_{\hat{b}_e}, \mathbf{u}_{\hat{b}_d}, \mathbf{u}_{\theta}$ can be computed analytically, and the GSA given in Eq. (61) becomes a double-loop procedure instead of a triple-loop procedure. The contribution of reducible uncertainty sources on the objective function can thus be quantified at a given $\mathbf{x}$.

The above discussed procedure only provides $S_{U_{g1}}^1(\mathbf{x})$ at a specific design setting $\mathbf{x}$. In order to check the quality of the surrogate model over the entire design region, the maximum value of $S_{U_{g1}}^1(\mathbf{x})$, $\mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u]$ need to be identified. A straightforward way of doing this is to perform GSA for all $\mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u]$. However, this is very computationally expensive. In this paper, the Efficient Global Optimization (EGO) method proposed by Jones et.al. [19] is employed to solve $\max_{\mathbf{x} \in [\mathbf{x}_l, \mathbf{x}_u]} \{S_{U_{g1}}^1(\mathbf{x})\}$. The main steps of EGO are briefly summarized as below:

- (1) Construct an initial Kriging model for $S_{U_{g1}}^1(\mathbf{x})$ as a function of $\mathbf{x}$.
- (2) Identify the location with the maximum Expected Improvement (EI) function. If the maximum EI satisfies the convergence criterion, stop and report the maximum $S_{U_{g1}}^1(\mathbf{x})$; otherwise, go to the next step.
- (3) Add the location with the maximum EI as the new training point for the Kriging surrogate model. Update the Kriging model and go to Step 2.

More details of the EGO method are available in Ref. [19]. For a black box function $S_{U_{g1}}^1(\mathbf{x})$, the EI function is defined as [19, 44]

$$EI_S(\mathbf{x}) = (-S^* + \hat{S}_{U_{g1}}^1(\mathbf{x}))F\left(\frac{(-S^* + \hat{S}_{U_{g1}}^1(\mathbf{x}))}{s_S(\mathbf{x})}\right) + s_S(\mathbf{x})f\left(\frac{(-S^* + \hat{S}_{U_{g1}}^1(\mathbf{x}))}{s_S(\mathbf{x})}\right), \quad (66)$$

where S^* is the current best solution, $\hat{S}_{U_{g1}}^1(\mathbf{x})$ is the Kriging mean prediction at location $\mathbf{x}$, $s_S(\mathbf{x})$ is the standard deviation of Kriging prediction, $f(\cdot)$ is the probability density function (PDF) of a standard normal variable.

After the maximum $\hat{S}_{U_{g1}}^1(\mathbf{x})$ is identified, we check whether it is less than a desired threshold (say 0.01). If it is satisfied, we perform CEDO. Otherwise, we add more training points near the design region with maximum $\hat{S}_{U_{g1}}^1(\mathbf{x})$ to improve the quality of the surrogate model of the simulation model.

3.5.2. Solution of the CEDO model

Since there is no explicit expression available for the CEDO objective function, we also use the EGO to solve the CEDO model given in Eq. (42). The EI function is defined as [19, 44]

$$EI_F(\mathbf{x}) = (F^* - \hat{F}(\mathbf{x}))F\left(\frac{(F^* - \hat{F}(\mathbf{x}))}{s_{\hat{F}}(\mathbf{x})}\right) + s_{\hat{F}}(\mathbf{x})f\left(\frac{(F^* - \hat{F}(\mathbf{x}))}{s_{\hat{F}}(\mathbf{x})}\right), \quad (67)$$

where F^* is the current best solution, $\hat{F}(\mathbf{x})$ is the Kriging mean prediction at location $\mathbf{x}$, $s_{\hat{F}}(\mathbf{x})$ is the standard deviation of Kriging prediction.

Based on the definition of the EI function, the new training point of the objective function surrogate model is identified in each of the iterations by maximizing the EI function. The maximum EI value is checked during each of the iterations. If the maximum EI satisfies a convergence criterion, the algorithm stops and the optimal solution is obtained. In this paper, the EGO method is used to solve the optimization model. The developed algorithm, however, is not limited to the EGO method. Other optimization algorithms can be employed as well.

In the next section, we will summarize the main implementation procedure of the proposed CEDO model with high-dimensional response and model uncertainty.

3.6. Implementation procedure

The implementation steps of the proposed CEDO method are summarized as below. There are mainly two modules, namely *surrogate modeling* and *design optimization*.

Module 1: Surrogate modeling

Step 1: Generate training points for experimental inputs $\mathbf{x}$ and calibration parameters $\boldsymbol{\theta}$ using Latin Hypercube Sampling (LHS) approach.

Step 2: Perform simulations at the training points and obtain the high-dimensional field response. Build surrogate models for the simulation model and discretization error using the method presented in Sec. 3.2.

Step 3: Check the quality of the surrogate modeling using the GSA-based method presented in Sec. 3.5.1. If the requirement is satisfied, go to next step. Otherwise, add more training points and go back to Step 2.

Module 2: Design optimization

Step 4: Generate training points for design variables $\mathbf{x}$ using the LHS approach.

Step 5: Compute the objective function at the training points using Eqs. (58) and (59), and the method presented in Sec. 3.4.

Step 6: Build a surrogate model for $F(\mathbf{x})$ and compute $EI_F(\mathbf{x})$ using Eq. (67).

Step 7: Check convergence of $EI_F(\mathbf{x})$. If convergence criterion is satisfied, obtain the optimal design $\mathbf{x}^*$. Otherwise, add the identified new training point $\mathbf{x}$ by maximizing $EI_F(\mathbf{x})$ and go to Step 5.

4. Numerical Examples

In this section, a nonlinear analytical example and a heat transfer example are used to illustrate the proposed method.

4.1. A nonlinear analytical example

A nonlinear function given in Eq. (68) is employed as our first example.

$$\begin{aligned} y_{obs}(z) &= G(x, \boldsymbol{\theta}) + d + e_{obs} \\ &= 50[\sin(x_{temp} z^2) - \cos(3(x_{temp} - z)^2 q_1^2) + (x_{temp} + q_2 - q_1 z)^2] + d + e_{obs}, \end{aligned} \quad (68)$$

where $\boldsymbol{\theta} = [q_1, q_2]$ are the calibration parameters, $x_{temp} = (3 + 3\sin(x + 6)) / (3 + \cos(4x - 0.5))$, z is the observation coordinate, $G(x, \boldsymbol{\theta})$ is the prediction model, e_{obs} is observation error, and x is the scalar experiment input that needs to be optimized. The model discrepancy d is assumed as

$$d(z) = 100 + 10(xz^2 + 2(\sin(2(x - z)))^2) \quad (69)$$

The observation errors at different spatial location are assumed to be identical and independent random variables given by $e_{obs} \sim N(0, 8^2)$. The prior distributions of $\boldsymbol{\theta} = [q_1, q_2]$ are assumed as $q_1 : N(0.8, 0.4^2)$ and $q_2 : \text{Unif}(0.8, 2.4)$. The range of the design variable is given by $x \in [0.1, 3]$. One experiment needs to be designed and 30 spatial observation locations over the domain of $z \in [0, 3.5]$ are used to collect the observation data for calibration. We first perform CEDO using the true models given in Eqs. (68) and (69). The weights of mean and variance are selected as $w_1 = w_2 = 0.5$. Fig. 3 plots the objective function with different experiment input settings. The result shows that the optimal design obtained from the true model is $x^* = 2.440$. To illustrate the proposed method, we assume that the prediction model $G(x, \boldsymbol{\theta})$ is expensive to evaluate. We therefore build a surrogate model for $G(x, \boldsymbol{\theta})$ to perform CEDO.

Fig. 3 Objective function evaluated based on the true model

(a) Surrogate modeling

We first generate 30 training points for x and θ using the LHS method. We then construct a surrogate model for $G(x, \theta)$ using the SVD-based Kriging method. At the same time, we assume that five experiments have been performed and a surrogate model is then built for the model discrepancy term. Fig. 4 shows the surrogate model of one latent response of $G(x, \theta)$ and its standard deviation.

Fig. 4 Mean prediction and standard deviation of a hidden response (for $x = 2$)

(b) Refining of surrogate model based on GSA

As discussed in Sec. 3.5.1, the surrogate model uncertainty may introduce extra uncertainty into the objective function, which will then affect the optimization result. In order to reduce the effect of surrogate model uncertainty, the GSA-based surrogate model checking method as presented in Sec. 3.5.1 is used here for the refinement of the surrogate model of $G(x, \theta)$. We identify the maximum first-order Sobol index in the design region using the method discussed in Sec. 3.5.1. Fig. 5 (a) shows that the maximum first-order Sobol index is larger than our requirement (0.01). We then add 20 new training points near the design point associated the maximum first-order Sobol index. After that, we identify the maximum first-order Sobol index again as shown in Fig. 5(b). We then add 25 new training points near the new maximum Sobol index point. After that, the requirement of GSA is satisfied. We then perform CEDO based on the refined surrogate model of $G(x, \theta)$. Note that the number of new training points is selected arbitrarily based on the computational effort that we can afford. Adaptively selecting training points one by one for the surrogate model of CEDO will be one of our future works.

In order to illustrate the effect of surrogate model refinements on the result of CEDO, we performed CEDO based on the initial surrogate model (30 training points), surrogate model after the 1st refinement (50 training points), and surrogate model after the 2nd refinement (75 training points), respectively. Fig. 6 gives the CEDO iteration history after the two refinements. Table 1 gives the optimal designs obtained during the refinement of the surrogate model. The results show that the optimal designs are getting closer to the true optimal design ($x^* = 2.440$) as the surrogate model gets more refined.

Fig. 5 First order Sobol index of the surrogate model uncertainty (before and after 1st refinement)

Fig. 6 CEDO after surrogate model refinements

Table 1 Optimal designs obtained during the refinements of the surrogate model

Number of Training Points	30	50	75	True
Optimal Design	2.51	2.49	2.435	2.440

(c) *Parametric study*

We first study the effects of the number of training points of the simulation model surrogate on the results of CEDO. Table 2 gives the optimal design of CEDO obtained from surrogate models built with different numbers of training points without using the GSA-informed refinement method. Of course, the optimal design will get closer to the true value ($x^* = 2.440$)

as more training points are used in the surrogate modeling. The results in Tables 1 and 2 show that 180 training points generated directly from LHS without using GSA-informed refinement method can achieve similar accuracy of CEDO obtained from surrogate model with 75 training points selected based on GSA. This demonstrates the effectiveness of the GSA-informed surrogate model refinement.

Table 2 Optimal designs obtained with different number of training points for the simulation model surrogate

Number of Training Points	30	50	75	120	150	180
Optimal design	2.51	2.475	2.411	2.41	2.419	2.436

We also studied the effect of model discrepancy on experiment design for this numerical example. Table 3 gives the optimal design obtained with and without model discrepancy term by directly generating training points using LHS. It shows that the effect of model discrepancy term on optimal design is minor for this problem. However, this phenomenon is problem-dependent.

Table 3 Optimal designs obtained with and without discrepancy

Number of Training Points	30	50	75	120	150	180
With discrepancy	2.51	2.475	2.411	2.41	2.419	2.436
Without discrepancy	2.503	2.474	2.411	2.40	2.419	2.436

4.2. A heat transfer problem

A cement slab ($15.5 \text{ in} \times 15.5 \text{ in} \times 1.75 \text{ in}$) as shown in Fig. 7 is used as our second example. This example is modified from the Sandia thermal challenge problem [45] by replacing the numerical equation with a finite element simulation model since FEA simulation can be applied for more complicated problems. The thermal conductivity (k) and volumetric heat capacity (ρC_p) of this cement slab need to be calibrated. In order to collect observation data for calibration, uniform heat flux is applied at the bottom of the slab, and the temperature on the top surface is measured at $16 \times 16 = 256$ observation locations (uniformly distributed on the top

surface) after a specified time interval. The experimental design variables include the duration T_{heat} that the heat flux is applied and the amplitude of heat flux q . The design ranges are given as

$$\begin{aligned} 1900 \text{ Secs} \leq T_{heat} \leq 3500 \text{ Secs}, \\ 0.001 \text{ Btu} / \text{in}^2 \text{ s} \leq q \leq 0.002 \text{ Btu} / \text{in}^2 \text{ s}. \end{aligned} \quad (70)$$

Fig. 7 A cement slab with heat flux applied on the bottom surface

The prior distributions of k and rC_p are assumed to be $k \sim \text{Unif}(4.42 \times 10^{-6}, 9.5 \times 10^{-6}) \text{ Btu} / (\text{s in}^\circ \text{F})$ and $rC_p \sim N(69, 5^2) \text{ Btu in} / \text{lbf s}^2 \text{ }^\circ \text{F}$.

Assuming for the sake of illustration that the computer simulation model of the cement slab is computationally expensive, we first construct surrogate models for the temperature field response at the top surface. The design variables of the surrogate model are $\mathbf{d} = [T_{heat}, q, k, rC_p]$.

4.2.1. Surrogate modeling

In order to build the surrogate model for the temperature field response at the top surface of the slab, 70 training points are generated first for q , T_{heat} , k , and rC_p using the LHS design method. At each training point, finite element simulation is performed using Abaqus [46] to obtain the temperature field response. The four edges of the slab are unconstrained. In the FEA simulation, the slab is meshed with a 3D continuum element in the Abaqus/Explicit FE library, a

coupled displacement-temperature 8 node solid element (C3D8T). Table 4 gives the material properties of the cement material used in the FEA simulation model.

Table 4 Material properties of the cement in simulation

Variable	Density	Young's modulus	Poisson's ratio	Film coefficient
Value	1990 kg/m ²	2.92 GPa	0.2	16.5 W/ m ² K

In order to account for the numerical discretization error of the simulation model, for each training point, the four edges of the top and bottom surfaces are first discretized into 15 elements in FEA simulation. Finer and finest FEA simulations are also performed for each of the training points by discretizing the four edges of the top and bottom surfaces into 30 and 60 elements. Fig. 8 shows the finite element model with the aforementioned three mesh sizes. Table 5 presents the number of nodes and elements in the three kinds of mesh-size simulation models.

Fig. 8 Finite element model with three different mesh sizes

Table 5 Number of nodes and elements in three different mesh size models

Case	1	2	3
No. of Nodes	1536	5766	22326
No. of Elements	1125	4500	18000

Fig. 9 (a) shows one example of the simulation model with mesh size case 1 and input variables $T_{heat} = 2415.2 \text{ Secs}$, $rC_p = 66.02 \text{ Btu in / lbf s}^2 \text{ } ^\circ F$, $q = 0.00149 \text{ Btu / in}^2 \text{ s}$, and $k = 8.877 \times 10^{-6} \text{ Btu / (s in } ^\circ F)$. Fig. 9 (b) gives corresponding estimated discretization error

quantified using the Richardson extrapolation method (Sec. 3.3.2). With all the temperature field responses and numerical discretization error responses at the training points, the SVD is then employed to decompose the high-dimensional field response into low dimensional latent responses.

Fig. 9 Simulation result at one training point and corresponding discretization error

Fig. 10 shows the first two important features (mode shapes or eigenfunctions of SVD) of the temperature response of the simulation model on the top surface of the slab for the case shown in Fig. 9. Fig. 11 shows the reconstructed temperature response using the first twenty important features for the case shown in Fig. 9. Fig. 11 (b) gives the difference (bias of the surrogate model) between the original and reconstructed responses. The maximum difference between the two is observed to be less than 0.05%, which implies that using the first twenty important features is accurate enough to model the temperature field response. Following the same procedure, a surrogate model is constructed for the numerical discretization error of the simulation model.

Based on SVD, Kriging models are then constructed for the latent responses, $\hat{b}_i(\mathbf{d})$, $i = 1, 2, \dots, 20$, and $\hat{b}_{e,j}(\mathbf{d})$, $j = 1, 2, \dots, 22$ (as discussed in Sec. 3.3). The obtained SVD-based surrogate models are then applied to the experimental design optimization. In order to illustrate

the advantage of the SVD-based Kriging surrogate modeling method, we compare the computational time required by the direct Kriging method and SVD-based Kriging method for one prediction. Table 6 gives the required computational time for these two types of surrogate models with different number of training points. It shows that the SVD-based Kriging method increases the computational efficiency and reduces the requirement of memory significantly for problems with field response.

Fig. 10 First two important features for the temperature response on the top surface of the slab

Table 6 Computational time of direct Kriging and SVD-based Kriging (one prediction)

Number of training points	5	10	15	50	70
Direct Kriging (Secs)	19.65	81.84	228.76	OM	OM
SVD-Kriging (Secs)	0.09	0.22	0.26	0.68	1.59

- “OM” is “out of memory”, the computational times were based on a laptop with Intel (R) Core (TM) i5-3230M CPU@2.60GHz and 4.00 GB system memory (RAM).

4.2.2. Experimental design optimization

Similar to Example 1, the observation noise term is assumed to be a Gaussian random variable given by $e_{obs} \sim N(0, 1)$ for the experimental design. The weights of mean and variance are selected as $w_1 = w_2 = 0.5$. After checking the quality of the surrogate models using the method proposed in Sec. 3.5, it shows that the maximum first order sensitivity index of the

surrogate model uncertainty is less than 0.01. We then perform CEDO using the surrogate models. Following the procedure given in Sec. 3.6, 4 initial training points are generated for the design variables T_{heat} and q . Based on the training points and corresponding values of the objective function, an initial surrogate model is constructed for the objective function. Fig. 12 gives the mean prediction and mean square error (MSE) of the objective function from the surrogate model after a new training point is added. The expected improvement (EI) (as shown in Fig. 13) is then computed based on the mean, MSE, and variances of the objective function.

Fig. 11 Comparison of original and reconstructed temperature response

Fig. 12 Mean prediction and MSE of the objective function after the 1st iteration

Based on the EI, the new training point is identified. The surrogate model of objective function is trained again with the updated training points and the EI function is computed again.

This procedure continues until the convergence criterion is satisfied. Fig. 14 gives the iteration history of the design variables. It indicates that the optimization converges after three iterations and the optimal point is identified as $T_{heat}^* = 3500$ Secs and $q^* = 0.002$ Btu / in²s .

Fig. 13 EI of the 2nd and 3rd iterations

Fig. 14 Iteration history of the design variables

The optimization results show that the optimal experimental parameters for Example 2 all go to the upper bounds of the design variables as given in Eq. (70).

5. Conclusion

Design optimization of calibration experiments aims to determine the optimal experimental input settings in order to generate the most valuable observations for model calibration. Current

experimental design methods mainly focus on problems with low-dimensional response and without considering model uncertainty. Model uncertainty is important to be included in CEDO since synthetic observation data are generated using a simulation model during the implementation of CEDO.

This paper developed a new method for experimental design optimization with field response in the presence of observation errors and model uncertainty including model discrepancy of the original simulation model, bias of the surrogate model, numerical discretization error, and prediction uncertainty of the surrogate model. The proposed method consists of two components: surrogate modeling of field response and experimental design optimization. An analytical method is developed to efficiently estimate the objective function. In order to check the quality of the surrogate model used in CEDO, a global-sensitivity analysis-based method is proposed to quantify the contribution of surrogate model uncertainty on the uncertainty of the objective function. Based on the above efforts, a new robust experimental design optimization model is formulated which is solved using the efficient global optimization method. A numerical example and a heat transfer example demonstrate the effectiveness of the proposed method.

The method presented in this paper only considered problems with one field response variable. Future extensions may consider problems with multiple field response variables with spatial and temporal observations. Experiments for effective calibration of model parameters that have spatial variability are also of interest, and need to be addressed in future work. Using the adjoint methods to improve the accuracy of experimental design optimization and adaptive sampling approach for surrogate modeling will be studied in future as well.

Acknowledgement

This study was partly supported by funds from the National Science Foundation (Grant No. 1404823, CDSE Program), and from the U. S. Department of Energy's Light Water Reactor Sustainability program at the Idaho National Laboratory, related to the effort on structural health monitoring of concrete components (project monitors: Bruce Hallbert, Vivek Agarwal). The support is gratefully acknowledged. The authors also thank Paromita Nath, graduate student at Vanderbilt University, for conducting the finite element simulations in the second numerical example.

Appendix A. Kriging Model

The output of a Kriging model is assumed to be a Gaussian stochastic process [47, 48]. The Kriging model of a black box function $g(\mathbf{d})$ is given by [47]

$$\hat{g}(\mathbf{d}) = \mathbf{h}(\mathbf{d})^T \mathbf{v} + \varepsilon(\mathbf{d}) \quad (\text{A1})$$

where $\mathbf{d}$ is the vector of input variables, $\mathbf{v} = [\nu_1, \nu_2, \dots, \nu_p]^T$ is a vector of unknown coefficients, $\mathbf{h}(\mathbf{d}) = [h_1(\mathbf{d}), h_2(\mathbf{d}), \dots, h_p(\mathbf{d})]^T$ is a vector of regression functions, $\mathbf{h}(\mathbf{d})^T \mathbf{v}$ is the trend of prediction, and $\varepsilon(\mathbf{d})$ is usually assumed to be a Gaussian process with zero mean and covariance $\text{Cov}[\varepsilon(\mathbf{d}_i), \varepsilon(\mathbf{d}_j)]$ given by

$$\text{Cov}[\varepsilon(\mathbf{d}_i), \varepsilon(\mathbf{d}_j)] = \sigma_\varepsilon^2 R(\mathbf{d}_i, \mathbf{d}_j) \quad (\text{A2})$$

in which σ_ε^2 is the process variance and $R(\cdot, \cdot)$ is the correlation function.

With n_s training points, $[\mathbf{d}_i, g(\mathbf{d}_i)]_{i=1, 2, \dots, n_s}$, the coefficients $\mathbf{v}$ are obtained by

$$\mathbf{v} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1} \mathbf{g} \quad (\text{A3})$$

where $\mathbf{R}$ is the correlation matrix with element, $R(\mathbf{d}_i, \mathbf{d}_j)$, $i, j = 1, 2, \dots, n_s$,

$\mathbf{H} = [\mathbf{h}(\mathbf{d}_1)^T, \mathbf{h}(\mathbf{d}_2)^T, \dots, \mathbf{h}(\mathbf{d}_{n_s})^T]^T$, and $\mathbf{g} = [g(\mathbf{d}_1), g(\mathbf{d}_2), \dots, g(\mathbf{d}_{n_s})]^T$.

For a new point $\mathbf{d}$, the mean of the prediction is given by

$$\hat{g}(\mathbf{d}) = \mathbf{h}(\mathbf{d})^T \mathbf{v} + \mathbf{r}(\mathbf{d})^T \mathbf{R}^{-1}(\mathbf{g} - \mathbf{H}\mathbf{v}) \quad (\text{A4})$$

$$\mathbf{r}(\mathbf{d}) = [R(\mathbf{d}, \mathbf{d}_1), R(\mathbf{d}, \mathbf{d}_2), \dots, R(\mathbf{d}, \mathbf{d}_{n_s})] \quad (\text{A5})$$

The mean square error (MSE) of the prediction is given by [49]

$$\begin{aligned} \text{MSE}(\mathbf{d}) = & \sigma_\varepsilon^2 \{1 - \mathbf{r}(\mathbf{d})^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{d}) \\ & + [\mathbf{H}^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{d}) - \mathbf{h}(\mathbf{d})]^T (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} [\mathbf{H}^T \mathbf{R}^{-1} \mathbf{r}(\mathbf{d}) - \mathbf{h}(\mathbf{d})]\} \end{aligned} \quad (\text{A6})$$

$$\sigma_\varepsilon^2 = \frac{(\mathbf{g} - \mathbf{H}\mathbf{v})^T \mathbf{R}^{-1} (\mathbf{g} - \mathbf{H}\mathbf{v})}{n_s} \quad (\text{A7})$$

More details about Kriging model method can be found in [47, 48], and a MATLAB Kriging toolbox is available in [49].

References

- [1] Ling, Y., Mullins, J., and Mahadevan, S., 2014, "Selection of model discrepancy priors in Bayesian calibration," *Journal of Computational Physics*, 276, pp. 665-680.
- [2] Huan, X., and Marzouk, Y., 2014, "Gradient-based stochastic optimization methods in Bayesian experimental design," *International Journal for Uncertainty Quantification*, 4(6).
- [3] Chaloner, K., and Verdinelli, I., 1995, "Bayesian experimental design: A review," *Statistical Science*, pp. 273-304.
- [4] Box, G. E., and Lucas, H., 1959, "Design of experiments in non-linear situations," *Biometrika*, pp. 77-90.
- [5] Bai, D., Kim, M., and Lee, S., 1989, "Optimum simple step-stress accelerated life tests with censoring," *Reliability, IEEE Transactions on*, 38(5), pp. 528-532.

- [6] Huan, X., and Marzouk, Y. M., 2013, "Simulation-based optimal Bayesian experimental design for nonlinear systems," *Journal of Computational Physics*, 232(1), pp. 288-317.
- [7] Long, Q., Scavino, M., Tempone, R., and Wang, S., 2013, "Fast estimation of expected information gains for Bayesian experimental designs based on Laplace approximations," *Computer Methods in Applied Mechanics and Engineering*, 259, pp. 24-39.
- [8] Long, Q., Scavino, M., Tempone, R., and Wang, S., 2015, "A Laplace method for under-determined Bayesian optimal experimental designs," *Computer Methods in Applied Mechanics and Engineering*, 285, pp. 849-876.
- [9] Ryan, E. G., Drovandi, C. C., Thompson, M. H., and Pettitt, A. N., 2014, "Towards Bayesian experimental design for nonlinear models that require a large number of sampling times," *Computational Statistics & Data Analysis*, 70, pp. 45-60.
- [10] Chowdhury, R., Rao, B., and Prasad, A. M., 2009, "High- dimensional model representation for structural reliability analysis," *Communications in Numerical Methods in Engineering*, 25(4), pp. 301-337.
- [11] Jia, G., and Taflanidis, A. A., 2013, "Kriging metamodeling for approximation of high-dimensional wave and surge responses in real-time storm/hurricane risk assessment," *Computer Methods in Applied Mechanics and Engineering*, 261, pp. 24-38.
- [12] Han, Z., Zimmerman, R., and Görtz, S., 2012, "Alternative Cokriging Method for Variable-Fidelity Surrogate Modeling," *AIAA journal*, 50(5), pp. 1205-1210.
- [13] Golub, G. H., and Reinsch, C., 1970, "Singular value decomposition and least squares solutions," *Numerische mathematik*, 14(5), pp. 403-420.
- [14] Hombal, V., and Mahadevan, S., 2013, "Surrogate modeling of 3D crack growth," *International Journal of Fatigue*, 47, pp. 90-99.

- [15] Litvinenko, A., Matthies, H. G., and El-Moselhy, T. A., 2013, "Sampling and low-rank tensor approximation of the response surface," Monte Carlo and Quasi-Monte Carlo Methods 2012, Springer, pp. 535-551.
- [16] Litvinenko, A., and Matthies, H. G., 2013, "Numerical Methods for Uncertainty Quantification and Bayesian Update in Aerodynamics," Management and Minimisation of Uncertainties and Errors in Numerical Aerodynamics, Springer, pp. 265-282.
- [17] Litvinenko, A., and Matthies, H., 2010, "Sparse data formats and efficient numerical methods for uncertainties quantification in numerical aerodynamics," ECCM IV: Solids, Structures and Coupled Problems in Engineering.
- [18] Berger, J. O., 2013, Statistical decision theory and Bayesian analysis, Springer Science & Business Media.
- [19] Jones, D. R., Schonlau, M., and Welch, W. J., 1998, "Efficient global optimization of expensive black-box functions," Journal of Global optimization, 13(4), pp. 455-492.
- [20] Kennedy, M. C., and O'Hagan, A., 2001, "Bayesian calibration of computer models," Journal of the Royal Statistical Society. Series B, Statistical Methodology, pp. 425-464.
- [21] Hershey, J. R., and Olsen, P., "Approximating the Kullback Leibler divergence between Gaussian mixture models," Proc. Acoustics, Speech and Signal Processing, 2007. ICASSP 2007. IEEE International Conference on, IEEE, pp. IV-317-IV-320.
- [22] Du, X., Sudjianto, A., and Chen, W., 2004, "An integrated framework for optimization under uncertainty using inverse reliability strategy," Journal of Mechanical Design, 126(4), pp. 562-570.
- [23] Chatterjee, A., 2000, "An introduction to the proper orthogonal decomposition," Current science, 78(7), pp. 808-817.

- [24] Golub, G. H., and Van Loan, C. F., 2012, Matrix computations, JHU Press.
- [25] Long, Q., Motamed, M., and Tempone, R., 2015, "Fast Bayesian optimal experimental design for seismic source inversion," *Computer Methods in Applied Mechanics and Engineering*, 291, pp. 123-145.
- [26] Espig, M., Hackbusch, W., Litvinenko, A., Matthies, H. G., and Zander, E., 2012, "Efficient analysis of high dimensional data in tensor formats," *Sparse Grids and Applications*, Springer, pp. 31-56.
- [27] Kennedy, M. C., and O'Hagan, A., 2001, "Supplementary details on Bayesian calibration of computer models," Internal Report. URL <http://www.shef.ac.uk/~st1ao/ps/calsup.ps>.
- [28] Demkowicz, L., Oden, J., and Strouboulis, T., 1984, "Adaptive finite elements for flow problems with moving boundaries. part I: Variational principles and a posteriori estimates," *Computer methods in applied mechanics and engineering*, 46(2), pp. 217-251.
- [29] Szabo, B., 1990, "The use of a priori estimates in engineering computations," *Computer Methods in Applied Mechanics and Engineering*, 82(1), pp. 139-154.
- [30] Szabó, B., and Babuška, I., 2011, *Introduction to finite element analysis: formulation, verification and validation*, John Wiley & Sons.
- [31] Babuška, I., and Rheinboldt, W. C., 1978, "A- posteriori error estimates for the finite element method," *International Journal for Numerical Methods in Engineering*, 12(10), pp. 1597-1615.
- [32] Zienkiewicz, O. C., and Zhu, J. Z., 1987, "A simple error estimator and adaptive procedure for practical engineering analysis," *International Journal for Numerical Methods in Engineering*, 24(2), pp. 337-357.

- [33] Richardson, L. F., 1911, "The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam," *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character*, 210, pp. 307-357.
- [34] Celik, I., and Karatekin, O., 1997, "Numerical experiments on application of Richardson extrapolation with nonuniform grids," *Journal of fluids engineering*, 119(3), pp. 584-590.
- [35] Ainsworth, M., and Oden, J. T., 1997, "A posteriori error estimation in finite element analysis," *Computer Methods in Applied Mechanics and Engineering*, 142(1), pp. 1-88.
- [36] Hombal, V., and Mahadevan, S., 2011, "Bias minimization in Gaussian process surrogate modeling for uncertainty quantification," *International Journal for Uncertainty Quantification*, 1(4).
- [37] Gilks, W. R., 2005, *Markov chain monte carlo*, Wiley Online Library.
- [38] Carpenter, J., Clifford, P., and Fearnhead, P., "Improved particle filter for nonlinear problems," *Proc. Radar, Sonar and Navigation, IEE Proceedings-*, IET, pp. 2-7.
- [39] Rosenblatt, M., 1952, "Remarks on a multivariate transformation," *The annals of mathematical statistics*, pp. 470-472.
- [40] Bücker, H. M., Corliss, G., Hovland, P., Naumann, U., and Norris, B., 2006, *Automatic differentiation: applications, theory, and implementations*, Springer Science & Business Media.
- [41] Haldar, A., and Mahadevan, S., 2000, *Probability, reliability, and statistical methods in engineering design*, John Wiley & Sons, Incorporated.
- [42] Stein, M., 1987, "Large sample properties of simulations using Latin hypercube sampling," *Technometrics*, 29(2), pp. 143-151.

- [43] Sobol, I. M., 2001, "Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates," *Mathematics and computers in simulation*, 55(1), pp. 271-280.
- [44] Hu, Z., and Du, X., 2015, "Mixed Efficient Global Optimization for Time-Dependent Reliability Analysis," *Journal of Mechanical Design*, 137(5), p. 051401.
- [45] McFarland, J., and Mahadevan, S., 2008, "Multivariate significance testing and model calibration under uncertainty," *Computer methods in applied mechanics and engineering*, 197(29), pp. 2467-2479.
- [46] Hibbitt, Karlsson, and Sorensen, 2001, *ABAQUS/standard user's Manual*, Hibbitt, Karlsson & Sorensen.
- [47] Rasmussen, C. E., 2006, "Gaussian processes for machine learning," The MIT Press, ISBN 0-262-18253-X.
- [48] Santner, T. J., Williams, B. J., and Notz, W., 2003, *The design and analysis of computer experiments*, Springer.
- [49] Lophaven, S. N., Nielsen, H. B., and Søndergaard, J., 2002, "DACE-A Matlab Kriging toolbox, version 2.0."