Stacking designs: designing multi-fidelity computer experiments with confidence

Chih-Li Sung †, Yi (Irene) Ji ‡, Tao Tang §, and Simon Mak ¶

Abstract. In an era where scientific experiments can be very costly, multi-fidelity emulators provide a useful tool for cost-efficient predictive scientific computing. For scientific applications, the experimenter is often limited by a tight computational budget, and thus wishes to (i) maximize predictive power of the multi-fidelity emulator via a careful design of experiments, and (ii) ensure this model achieves a desired error tolerance with confidence. Existing design methods, however, do not jointly tackle objectives (i) and (ii). We propose a novel stacking design approach which addresses both goals. Using a recently proposed multi-level Gaussian process emulator model, our stacking design provides a sequential approach for designing multi-fidelity runs such that a desired prediction error of $\epsilon > 0$ is met under regularity conditions. We then prove a novel cost complexity theorem which, under this multi-level Gaussian process emulator, establishes a bound on the computation cost (for training data simulation) needed to ensure a prediction bound of $\epsilon$. This result provides novel insights on conditions under which the proposed multi-fidelity approach improves upon a standard Gaussian process emulator which relies on a single fidelity level. Finally, we demonstrate the effectiveness of stacking designs in a suite of simulation experiments and an application to finite element analysis.

Key words. Computer Experiments, Experimental Design, Finite Element Analysis, Gaussian Process Modeling, Multi-level Modeling, Uncertainty Quantification.

AMS subject classifications. 00A20

1. Introduction. With recent developments in scientific computing and mathematical modeling, computer experiments have now become an essential tool in solving many scientific and engineering problems. These experiments, which typically solve complex mathematical models representing reality, are useful in applications which are prohibitively expensive or infeasible for direct experimentation. Such virtual experiments have now been successfully applied in a broad range of problems, from nuclear physics [9] to rocket design [25]. As the science becomes more sophisticated, however, such simulations can become prohibitively costly for parameter space exploration. A popular solution is emulation [34], which makes use of a carefully designed training set from the simulator to build an efficient predictive model that emulates the expensive computer code. Popular emulator models include the Gaussian process (GP) model [33, 6, 13], neural networks [38, 28] and polynomial chaos methods [46], all of which have demonstrated successes in various areas of application. In the following, we will focus on GP-based emulators.

For full-scale complex scientific systems, however, it is often the case that the training data needed to train an accurate emulator model can be prohibitively expensive to generate from
the simulator. One way to address this is via multi-fidelity emulation, which supplements the costly high-fidelity (or high-accuracy) simulation dataset with less expensive lower-fidelity (or lower-accuracy) approximations for fitting the emulator model. The idea is that, by leveraging useful information from cheaper lower-fidelity simulations to enhance predictions for the high-fidelity model, an accurate multi-fidelity emulator can be trained with fewer high-fidelity runs and thus lower simulation costs. The usefulness of this multi-fidelity emulation framework has led to much work in recent years. A popular framework is the Kennedy-O’Hagan (KO) model [19], which models a sequence of computer simulations from lowest to highest fidelity using a sequence of Gaussian process (GP) models linked by a linear autoregressive framework. Recent developments on the KO model include [31, 20, 22, 21, 29, 17] (among many others), which investigated modeling strategies for efficient posterior prediction and Bayesian uncertainty quantification. For multi-fidelity simulators controlled by a single mesh parameter (e.g., mesh density in finite element analysis), [41] proposed a non-stationary GP model which leverages data at different mesh densities to predict the highest-fidelity simulation at the finest mesh. This has been further developed in subsequent works for multi-stage emulation [18] and black-box optimization [15].

Despite this body of work, there remains important unresolved needs, particularly on the design of such multi-fidelity experiments for cost-efficient emulation. In modern scientific computing problems, the experimenter is often limited by a tight computational budget dictated by available computing resources for a project; see, e.g., [3]. Given such constraints, one thus wishes to (i) maximize predictive power of the multi-fidelity emulator via a careful design of experiments, and (ii) ensure the resulting emulator achieves a desired prediction error bound with confidence. This allows for verifiable and cost-efficient emulation, which then translates to precise scientific inference given a computational budget. Despite its importance, however, there is little work to our knowledge on design methods for multi-fidelity emulators which jointly tackles objectives (i) and (ii). We thus propose a novel stacking design framework which aims to jointly address (i) and (ii).

In what follows, we let $f_l(x)$ denote the scalar (deterministic) simulation output of the computer code with input parameters $x \in \Omega \subseteq \mathbb{R}^d$ and at fidelity level $l$. In finite element analysis (FEA), this fidelity level may reflect the underlying mesh density of the numerical simulator. We further suppose that, as fidelity level $l$ increases, the simulated output $f_l(x)$ approaches a limiting solution of $f_\infty(x)$, the desired “exact” solution of the simulator. In practice, this exact solution often cannot be simulated numerically; for example, the limiting solution for finite element analysis (i.e., at an infinitely dense mesh density) often cannot be computed numerically. Our proposed method makes use of a recent Multi-Level GP (MLGP) emulator model in [7], which leverages simulated data of multiple fidelities to train a GP emulator for predicting the desired limiting solution $f_\infty(x)$.

With the MLGP emulator, the proposed stacking design aims to carefully choose the multi-fidelity experimental runs, such that a desired prediction bound of $\epsilon > 0$ is ensured between the MLGP predictor and the desired solution $f_\infty(\cdot)$. This is achieved by iterating the following sampling steps. First, for a fixed number of sampled fidelity levels $L$, we show that the MLGP provides an easy-to-evaluate expression for allocating sample sizes over each fidelity level. After performing runs with these sample sizes in a space-filling fashion, we then derive a novel stopping rule for deciding, under regularity conditions, whether the number of levels
\( L = 1 \)
\( x_1 \) (pressure side)
\( x_2 \) (suction side)
\( L = 2 \)
\( x_1 \) (pressure side)
\( x_2 \) (suction side)
\( L = 3 \)
\( x_1 \) (pressure side)
\( x_2 \) (suction side)
\( L = 4 \)
\( x_1 \) (pressure side)

Figure 1. Visualizing the stacking behavior of the proposed stacking designs for a jet engine turbine blade application investigated later. (Top) The proposed stacking designs at \( L = 4 \) fidelity levels, over four sequential design stages (from left to right). (Bottom) The corresponding sample sizes at the \( L = 4 \) fidelity levels, over four sequential design stages (from left to right).

\( L \) is sufficiently large for achieving the desired error bound \( \epsilon \). If \( L \) is not large enough, we then increment \( L \) and repeat the above design step. The resulting sequential design procedure creates a “stacking” effect, where design points are stacked on at each fidelity level until the stopping rule is satisfied, at which point the desired prediction bound \( \epsilon \) is satisfied under regularity conditions. This stacking behavior is visualized in the bottom of Figure 1, where we see the “stacking” of sample sizes at each fidelity stage as the sequential design progresses.

The proposed stacking designs are inspired by a similar sequential approach for multi-level Monte Carlo (MLMC; see [11]), which aims to provide cost-efficient error control for multi-level Monte Carlo simulations. We then demonstrate the effectiveness of the proposed stacking designs (in terms of cost efficiency and error guarantees) in a suite of simulation experiments and an application to finite element analysis.

A key novelty of our work is a new cost complexity theorem which, under the MLGP model, establishes a bound on the required computation cost (for training data generation) needed to ensure the desired prediction bound \( \epsilon \). Such a result sheds useful insight on when multi-fidelity emulation may be most (or least) effective given a computation cost budget. As a corollary, we then show that the presented multi-fidelity approach yields provably improved predictions over a standard single-fidelity GP emulator, under intuitive conditions on the error decay and cost complexity of the multi-fidelity simulator. These results are again inspired by existing work in MLMC for characterizing the cost complexity of multi-level Monte Carlo estimators.
To our knowledge, there has been little work on extending such results for characterizing cost complexity of multi-fidelity computer experiments; we aim to address this gap here.

The paper is organized as follows. Section 2 introduces the MLGP emulator model in [7]. Section 3 presents the proposed stacking designs in several steps. Section 4 discusses a cost complexity theorem for the MLGP. Section 5 investigates the effectiveness of stacking designs via a suite of simulation studies and an application to FEA. Section 6 concludes the paper. Proofs and code for reproducing numerical results are provided in Supplemental Materials.

2. Multi-Level Surrogate Modeling. We first introduce the multi-level Gaussian process emulator recently proposed in [7], which we leverage later for our stacking designs. Again, let \( f_l(x) \) denote the scalar simulation output of the computer code, with input parameters \( x \in \Omega \subseteq \mathbb{R}^d \) and at fidelity level \( l \). In what follows, we assume that \( L \) distinct fidelity levels have been sampled for training data, where a larger fidelity level indicates a higher fidelity (or higher accuracy) simulator with higher computational costs per run.

The goal then is to construct an efficient surrogate model, with uncertainty quantification, for the highest-fidelity (and thus most expensive) simulation code \( f_L(x) \). Suppose, for \( l \)-th fidelity level, simulations are performed at the design points \( X_l = \{ x^{[l]}_i \}_{i=1}^{n_l} \), where the sample size \( n_l \) varies for different fidelity levels \( l \). This yields the simulation outputs \( f|_{X_l} = (f_l(x))_{x \in X_l} \), where \( f|_{X} \) denotes the vector of outputs for \( f(x) \) at design points \( x \in \mathcal{X} \). For this multi-level emulator, we further assume that the designs \( X_l \) are sequentially nested, i.e.,

\[
X_L \subseteq X_{L-1} \subseteq \cdots \subseteq X_1 \subseteq \Omega,
\]

In other words, design points run for a higher fidelity simulator will be contained within the design points run for a lower fidelity simulator.

With this, the multi-level Gaussian process (MLGP) surrogate model from [7] is constructed as follows. Note that the high-fidelity response surface \( f_L \) can be decomposed as \( f_L = \sum_{l=1}^{L} (f_l - f_{l-1}) \), where \( f_0 \equiv 0 \). A probabilistic surrogate model for \( f_L \) can be formulated as:

\[
f_L(x) = \sum_{l=1}^{L} Z_l(x).
\]

Here, \( Z_l = f_l - f_{l-1} \) can be viewed as the discrepancy between the \((l-1)\)-th and \(l\)-th code, capturing refinements in the response surface as fidelity increases. One can thus view the model (2.2) as the telescoping sum of refinements from the \(L\) fidelity levels of the simulator.

Of course, the refinement functions \( Z_l \) are unknown prior to data. We adopt a Bayesian perspective and place independent zero-mean Gaussian process (GP) priors [34] on these functions:

\[
Z_l(x) \overset{\text{indep.}}{\sim} \mathcal{GP}\{0, \tau_l^2 \Phi_l(x, x')\}, \quad l = 1, \ldots, L,
\]

where \( \tau_l^2 \) is a variance parameter and \( \Phi_l(x, x') \) is a positive-definite kernel function. The resulting model on \( f_L(x) \) has some similarities to the co-kriging models in [19, 22, 21], which also assumes nested designs but models instead the function \((f_l - \rho_{l-1} f_{l-1})|_{X_l}\) via a GP prior, where \( \rho_{l-1} \) is an unknown parameter. One advantage of the above multi-level emulator
compared to co-kriging models, as discussed in [7], is that it explicitly models for the bias between the exact simulation solution and its surrogate model, thus allowing for quantifying the emulation accuracy in theory, which is developed in the next section.

As with standard GP emulators, a key advantage of the MLGP model in [7] is that its posterior predictive distribution can be evaluated as efficient, closed-form expressions. Specifically, for a new input $x$, the posterior distribution of each refinement $Z_l(x)$ given the data $z_l := (f_l - f_{l-1})|X_l$ can be shown to be normally distributed as:

$$Z_l(x) | z_l \sim N \left\{ \Phi_l(x, X_l) \Phi_l^{-1} z_l, \tau_l^2 \left( \Phi_l(x, x) - \Phi_l(x, X_l) \Phi_l^{-1} \Phi_l(x, X_l)^T \right) \right\},$$

where $\Phi_l(x, X_l) = \{\Phi_l(x, y)\}_{y \in X_l}$ and $\Phi_l = [\Phi_l(x_i^l, x_j^l)]_{i,j=1,...,n_l}$ for $l = 1, \cdots, L$. With this, the posterior predictive distribution of the highest-fidelity response surface $f_L$ is then given by:

$$(2.4) \quad f_L(x) | z_1, \ldots, z_L \sim N \left( \sum_{l=1}^L \Phi_l(x, X_l) \Phi_l^{-1} z_l, \sum_{l=1}^L \tau_l^2 \left( \Phi_l(x, x) - \Phi_l(x, X_l) \Phi_l^{-1} \Phi_l(x, X_l)^T \right) \right).$$

Details on this derivation can be found in [7]. The posterior mean in (2.4) then serves as an emulator for the high-fidelity response surface $f_L(x)$, and the posterior variance in (2.4) quantifies the uncertainty in this prediction. Note that both the posterior mean and variance can be efficiently computed over each fidelity level $l = 1, \cdots, L$.

In the following, we make use of the Matérn kernel $\Phi_l(x_i, x_j) = \phi_{\nu_l}(\Theta_l(x_i - x_j))$, where:

$$(2.5) \quad \phi_{\nu_l}(d) = \frac{2^{1-\nu_l}}{\Gamma(\nu_l)} \left( \frac{d}{2^{\nu_l}} \right)^{\nu_l} B_{\nu_l} \left( \frac{d}{2^{\nu_l}} \right).$$

Here, $\nu_l > 0$ is a smoothness parameter which controls differentiability of sample paths, $\Theta_l$ is a diagonal $d \times d$ matrix of lengthscales parameters, $B_{\nu_l}$ is the modified Bessel function of the second kind, and $\Gamma$ is the gamma function. Matérn kernels are widely used in the computer experiment [34, 13] and spatial statistics [36] literature, and we will show later that such a kernel choice yields useful insights for characterizing the cost complexity performance of stacking designs.

Of course, the model hyperparameters $\Theta_l, \nu_l$ and $\tau_l^2$ are unknown in practice and need to be estimated. One approach is via maximum likelihood estimation. One can show that the log-likelihood of these hyperparameters is given by:

$$(2.6) \quad -\frac{1}{2} \log 2\pi - \frac{1}{2} \log \tau_l^2 - \frac{1}{2} \log \det(\Phi_l) - \frac{1}{2\tau_l^2} z_l^T \Phi_l^{-1} z_l,$$

so their maximum likelihood estimates can be obtained by maximizing (2.6). Alternate parameter estimation approaches include cross-validation or fully Bayesian inference; we refer the reader to [5] and [32] for further details, with extensive numerical comparisons in [30]. It should be noted that, while the smoothness parameter $\nu_l$ is often specified as $\nu_l = \kappa + 1/2$ for a positive integer $\kappa$ in the literature [36, 13] (since such kernels can be computed more efficiently), recent papers (see, e.g., [39] and [30]) have raised concerns of
misspecified smoothness parameters for prediction accuracy. To this end, we adopt a similar approach to [30], which finds the maximum likelihood estimates for $\Theta_l$ and $\tau_l^2$ by fixing a grid of $\nu_l$ values, then using leave-one-out cross-validation to select the best choice for $\nu_l$ at each level $l$.

3. Stacking designs for MLGP emulator. With the MLGP in hand, we now introduce the proposed stacking designs. We first define some notation. Let $\mathcal{N}_\Phi(\Omega)$ be the reproducing kernel Hilbert space (RKHS, [43]) associated with a kernel $\Phi$, and let $\|g\|_{\mathcal{N}_\Phi(\Omega)}$ denote its RKHS norm for a function $g \in \mathcal{N}_\Phi(\Omega)$. In the following, we investigate an error bound on the posterior mean in (2.4), namely:

$$f_L(x) = \sum_{l=1}^{L} \Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} z_l.$$ 

This is used as the emulator for the multi-level model, and we thus refer to this as the MLGP emulator. It is worth noting that each term within the summation in (3.1), i.e., $\Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} z_l$, can be viewed as the RKHS interpolator [43, 14] of $(f_l - f_{l-1})|_{\mathcal{X}_l}$ using kernel $\Phi_l$.

Suppose, for each fidelity level $l$, there corresponds a measure of fidelity $\xi_l > 0$ quantifying how close the simulated response surface $f_l(\cdot)$ is to the exact solution $f_\infty(\cdot)$, which we denote as $f_\infty(\cdot)$. As $l \to \infty$, it is intuitive that $\xi_l \to 0$, meaning we approach the limiting solution as fidelity level increases. However, the exact solution $f_\infty(\cdot)$ typically cannot be computed numerically and must be approximated. In the case of finite element method (FEM), which is widely used for computer experiments, one such parameter for $\xi_l$ is the mesh size: a smaller mesh size $\xi_l$ results in higher mesh density and thus a more accurate simulator, at the cost of higher computation.

We now decompose the error in approximating the desired exact solution $f_\infty(x)$ with the MLGP predictor $\hat{f}_L(x)$ in (3.1). By the triangle inequality, this error bound can be decomposed as

$$|f_\infty(x) - \hat{f}_L(x)| \leq |f_\infty(x) - f_L(x)| + |f_L(x) - \hat{f}_L(x)|.$$ 

The first term corresponds to the simulation error, which measures the discrepancy between the simulated solution $f_L(x)$ at fidelity level $L$ and the ground truth $f_\infty(x)$. This error can be reduced by increasing $L$, the fidelity level $L$ of the simulator, or equivalently by reducing $\xi_l$. The second term represents emulation error - the error for the MLGP predictor given limited evaluations of the simulator $f_L(\cdot)$. This error can be reduced by increasing $n_L$, the sample size at the fidelity level $L$, or increase $n_{L-1}, \cdots, n_1$, the sample sizes at lower fidelity levels.

With this, the proposed stacking designs aim to develop a design scheme which guarantees the desired prediction accuracy of $\epsilon > 0$, i.e., $\|f_L - \hat{f}_L\| < \epsilon$. Here, $\|\cdot\|$ may be the $L_2$ or $L_\infty$ norm. This can be achieved by making both the simulation and emulation errors smaller than $\epsilon/2$, i.e.,

$$\|f_\infty - f_L\| < \epsilon/2 \quad \text{and} \quad \|f_L - \hat{f}_L\| < \epsilon/2.$$ 

We thus propose our stacking designs in two parts. In Section 3.1, we first present a sample size determination approach which bounds the emulation error $\|f_L - \hat{f}_L\|$ via closed-form
expressions for sample sizes at each fidelity level. In Section 3.2, we then present a useful stopping rule on the maximum fidelity L such that the simulation error bound on \( |f_{\infty} - \hat{f}_L| \) is satisfied. We then discuss a sequential algorithm for stacking designs in Section 3.3, and prove a novel complexity theorem guaranteeing its performance in Section 4.

### 3.1. Emulation error control

Consider first the emulation error \( |f_L - \hat{f}_L| \). We first present a useful bound on this error for the MLGP model (proof in Supplementary Material S1).

**Proposition 3.1.** Suppose \( \Omega \) is bounded and convex, and \( (f_l - f_{l-1}) \in \mathcal{N}_{\phi_l}(\Omega) \). Then one can bound the prediction error of \( \hat{f}_L(x) \) as:

\[
|f_L(x) - \hat{f}_L(x)| \leq c_0 \sum_{l=1}^{L} \|\Theta_l\|^2 \frac{h_{\mathcal{X}_l}^{\nu_l}}{\|\Phi_l\|^2} \|f_l - f_{l-1}\|_{\mathcal{N}_{\phi_l}(\Omega)}
\]

for some constant \( c_0 > 0 \). Here, \( h_{\mathcal{X}_l} \) is the fill distance \([43]\) of the design \( \mathcal{X}_l \), i.e., \( h_{\mathcal{X}_l} = \sup_{x \in \Omega} \min_{x_u \in \mathcal{X}_l} \|x - x_u\|_2 \).

This proposition nicely decomposes the prediction error of the MLGP emulator into three distinct components at each fidelity level \( l = 1, \ldots, L \). The first term, \( \|f_l - f_{l-1}\|_{\mathcal{N}_{\phi_l}(\Omega)} \), captures the size of the refinement with respect to its corresponding RKHS norm. This is quite intuitive, since a larger norm of the refinement \( f_l - f_{l-1} \) is expected to induce greater error. The second term, \( h_{\mathcal{X}_l}^{\nu_l} \), measures the quality of the design \( \mathcal{X}_l \) in terms of how well it fills the design space \( \Omega \). Note that a smaller fill distance \( h_{\mathcal{X}_l} \) suggests that there are less “gaps” between design points \([24]\), which in turn should reduce prediction error. The third term, \( \|\Theta_l\|^2 \), captures the magnitude of the lengthscales \( \Theta_l \). Larger lengthscale parameters result in wigglier sample paths from the MLGP, which in turn increases prediction error. These three components provide the basis for the stacking sequential design method presented next.

We now wish to minimize the error bound in (3.4) under a total budget on computational resources, to yield easy-to-evaluate expressions for determining sample sizes \( n_l \) at each fidelity level \( l = 1, \cdots, L \). Let \( C_l \) be the computational cost (e.g., in CPU hours) for a single run of the simulator at fidelity level \( l \). Note that, since higher-fidelity simulators are more computationally intensive, this implies that \( 0 < C_1 < C_2 < \ldots < C_L \).

From the experimental design perspective, an appealing design criterion for GP emulation is quasi-uniformity, which ensures design points are uniformly placed over the design space \( \Omega \). In particular, a design \( \mathcal{X} = \{x_i\}_{i=1}^n \) with such a property satisfies the fill distance bound \([43, 27]\) \( h_{\mathcal{X}} \leq c_1 n^{-1/d} \) for some constant \( c_1 > 0 \), where \( n \) is the number of design points in \( \mathcal{X} \). Quasi-uniformity has been widely studied in the literature \([10]\), and there are a variety of designs which enjoy this property \([45]\). We thus restrict the designs \( \mathcal{X}_l \) to be quasi-uniform for \( l = 1, \cdots, L \). The construction of such designs is discussed later in Section 3.3. Under this restriction, the error bound in (3.4) reduces to

\[
|f_L(x) - \hat{f}_L(x)| \leq c_0 C_1 \sum_{l=1}^{L} \|\Theta_l\|^2 n_l^{\nu_l - 1/d} \|f_l - f_{l-1}\|_{\mathcal{N}_{\phi_l}(\Omega)}.
\]

Consider now the sample size determination problem, where we wish to minimize the error bound in (3.5) under the constraint of the total computational budget, \( \sum_{l=1}^{L} n_l C_l \). This can
be done by the method of Lagrange multipliers, which aims to minimize:

\[
\sum_{l=1}^{L} \left( \|\Theta_l\|^\nu_l n_l^{-\nu_l/d} \|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)} + \lambda n_l C_l \right),
\]

where \( \lambda > 0 \) is the Lagrange multiplier. With some algebraic manipulations (by setting the gradient of the above function to zero), one can show that the optimal sample size for \( n_l \) is:

\[
n_l = \mu \left( \frac{\|\Theta_l\|^\nu_l}{C_l} \|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)} \right)^{d/(\nu_l + d)}
\]

for some constant \( \mu > 0 \).

The closed-form expression (3.6) reveals several useful insights for sample size determination in multi-fidelity experiments. First, with all things equal, we see that (3.6) allocates greater sample size \( n_l \) for simulations with lower costs \( C_l \) (i.e., lower fidelity simulations), which is intuitive. Second, note that (3.6) assigns greater sample size \( n_l \) for fidelity levels where the refinement \( f_l - f_{l-1} \) is more complex, whether that be in terms of a larger lengthscale \( \Theta_l \) or a larger RKHS norm. In particular, note that the RKHS norm of \( f_l - f_{l-1} \) captures dissimilarities of the simulators from fidelity level \( l - 1 \) to level \( l \). Thus, by minimizing (3.6), our approach naturally factors in this dissimilarity information for optimal sample size allocation.

There is still a free constant \( \mu \), which we can set to achieve the desired emulation error \( \|f_L - \hat{f}_L\| < \epsilon/2 \). This parameter can be optimized as follows. By Theorem 11.14 of [43], an alternative pointwise error bound of \( \hat{f}_L(x) \) is

\[
|f_L(x) - \hat{f}_L(x)| \leq \sum_{l=1}^{L} \sigma_l(x)\|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)},
\]

where \( \sigma_l(x) \) is the so-called power function of the form

\[
\sigma_l^2(x) = \Phi_l(x, x) - \Phi_l(x, \mathcal{X}_l)\Phi_l^{-1}\Phi_l(x, \mathcal{X}_l)^T.
\]

In contrast from the error bound in Theorem 3.1, the bound (3.7) does not depend on any constants, which allows for the following development. By the triangle inequality, \( \|f_L - \hat{f}_L\| \) can be bounded by

\[
\|f_L - \hat{f}_L\| \leq \sum_{l=1}^{L} \|\sigma_l\|\|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)}.
\]

To ensure the bound in (3.9) is less than the desired error tolerance \( \epsilon/2 \), one can set the constant \( \mu \) by solving the optimization problem

\[
\mu^* = \arg\min_{\mu > 0} \left( \frac{\epsilon}{2} - \sum_{l=1}^{L} \|\sigma_l\|\|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)} \right) \text{ s.t. } \sum_{l=1}^{L} \|\sigma_l\|\|f_l - f_{l-1}\|_{\mathcal{N}_{\nu_l}(\Omega)} < \frac{\epsilon}{2}.
\]

Here, the dependency of the objective function on \( \mu \) is via the term \( \|\sigma_l\| \). This is because \( \sigma_l(x) \) depends on the sample size \( n_l \) and subsequently \( \mu \) (recall \( n_l = \lfloor \mu r_l \rfloor \)), since the power function
depends on the design points \( X \). To optimize for \( \mu^* \) in (3.10), \( \| \sigma_l \| \) can be approximated numerically via Monte Carlo integration [2] for \( L_2 \) norm and grid search optimization for \( L_\infty \) norm.

Finally, to optimize \( \mu^* \), we also require knowledge of the RKHS norm \( \| f_l - f_{l-1} \|_{\mathcal{H}}(\Omega) \). Of course, the exact norm is unknown in implementation since it depends on \( f_l \) and \( f_{l-1} \). One can, however, approximate this term via its RKHS interpolator, which can be shown to equal \( (z_l^T \Phi_l^{-1} z_l)^{1/2} \) [43]. Similarly, the kernel parameters \( \Theta_l \) and \( \nu_l \), which are also required for the optimization, can also be adaptively estimated via maximum likelihood and cross-validation as mentioned in Section 2. With these plug-in estimates within (3.10), the desired \( \mu^* \) can then be efficiently obtained via grid search or gradient-free optimization algorithms.

We note that the above sample size determination approach has several key distinctions from that in [7]. First, our proposed sample sizes are determined by the desired prediction accuracy \( \epsilon \) via (3.10), while theirs are controlled by a fixed total cost budget. This becomes important in the following subsection, where we leverage such sample sizes within a sequential stacking approach for controlling prediction error. Second, our approach makes use of an initial pilot sample (called \( X_0 \) later) to estimate the RKHS norm and other required parameters in (3.6), which lends well to our later sequential design procedure. The approach in [7], by contrast, makes use of misspecified kernel functions, in particular, the rates proved in [42].

### 3.2. Simulation error control via stacking

Consider next the simulation error \( \| f_\infty - f_L \| \) in (3.3), which concerns the numerical error of the simulator at fidelity level \( L \). For many numerical simulators, this error can be bounded as

\[
|f_\infty(x) - f_l(x)| \leq c_1 \xi_l^\alpha, \quad \text{for all } x \in \Omega,
\]

for some positive constants \( c_1 \) and \( \alpha \). Recall that \( \xi_l \) is a fidelity parameter which quantifies how close \( f_l(\cdot) \) is to the exact solution \( f_\infty(\cdot) \); the smaller \( \xi_l \) is, the higher the fidelity of the simulator \( f_l(\cdot) \). Equation (3.11) thus assumes that the simulation error is decaying polynomially in the fidelity parameter \( \xi_l \). In the case of FEM with \( \xi_l \) taken as the finite-element mesh size, it is well-known that the bound (3.11) holds under regularity conditions on the underlying solution (see, e.g., [1, 41]). Similarly polynomial decay rates have also been shown in a broad range of numerical simulators, e.g., for elliptical PDEs [16] and large-eddy simulations in fluid mechanics [37]. We will thus assume the error bound in (3.11), and leverage this for controlling simulation error via the stacking designs presented next.

Suppose the fidelity parameters \( \{ \xi_1, \xi_2, \cdots \} \) follow a geometric sequence for increasing fidelity levels, i.e., \( \xi_l = \xi_0 T^{-l}, l \in \mathbb{N}^+ \) for some integer \( T \geq 2 \). In the setting of FEM, where \( \xi_l \) measures finite-element mesh size, \( \xi_1, \xi_2, \cdots \) correspond to mesh sizes for increasing mesh refinements. The use of such a geometric sequence is motivated by multilevel Morte Carlo (MLMC) [11, 12], which makes use of a similar sequence for time discretization of stochastic differential equations.

We now wish to ensure the simulation error satisfies the desired bound of \( \| f_\infty - f_L \| < \epsilon/2 \). Using the above sequence and the assumed error bound (3.11), we have

\[
|f_\infty(x) - f_l(x)| \approx c_1 \xi_l^\alpha = c_1 \xi_0^\alpha T^{-\alpha l}, \quad l = 1, \cdots, L.
\]
With some algebraic manipulations, we can then show that

\[ |f_l(x) - f_{l-1}(x)| \approx c_2 T^{-\alpha_l}, \quad l = 2, \ldots, L, \]

for some positive constant \( c_2 \). The desired numeric error is then be bounded by

\[
|f_\infty(x) - f_L(x)| \leq \sum_{l=L+1}^{\infty} |f_l(x) - f_{l-1}(x)| \approx |f_L(x) - f_{L-1}(x)| \sum_{l=1}^{\infty} T^{-\alpha_l}
\]

\[
= \frac{|f_L(x) - f_{L-1}(x)|}{T^{\alpha} - 1} := b(x).
\]

(3.13)

Of course, the numerator \( |f_L(x) - f_{L-1}(x)| \) is unknown in implementation; we can, however, estimated it via its posterior mean from the MLGP, namely, \( |\Phi_L(x, \mathcal{X}_L)\Phi_L^{-1}z_L| \). Combining everything together, the following criterion then serves as a check for whether the desired simulation error bound is met \( \|f_\infty - f_L\| < \epsilon/2 \),

\[
\frac{\|\Phi_L(x, \mathcal{X}_L)\Phi_L^{-1}z_L\|}{T^{\alpha} - 1} < \frac{\epsilon}{2}.
\]

(3.14)

The above procedure extends a similar argument made in [11] for bounding approximation error in MLMC.

From (3.14), one sees that the rate parameter \( \alpha \) plays an important role for ensuring \( \|f_\infty - f_L\| < \epsilon/2 \). One way to set this parameter, as suggested in [41], is to infer \( \alpha \) via the known error bound (3.11) from numerical analysis. For example, in FEM, if the interest lies in the integration of \( f(x) \) over a specific region, then \( \alpha = 2 \) is suggested [41]. If such prior information is not available from numerical analysis, then one could instead estimate this rate from data. In particular, using the approximation in (3.12), one can use the simulated data \((f_l - f_{l-1})|_{\mathcal{X}_l}, \ l = 2, \ldots, L\) and estimate \( \alpha \) via linear regression with a log-transformation on the response.

3.3. Stacking design algorithm. We now combine the two error control approaches in Sections 3.1 and 3.2 into a sequential algorithm for stacking designs. From previous developments, there are two key properties that the design points in \( \mathcal{X}_l, \ l = 1, \ldots, L \), should satisfy: (i) they should be nested over fidelity levels, i.e., \( \mathcal{X}_1 \subseteq \cdots \subseteq \mathcal{X}_L \), and (ii) for each fidelity level \( l \), the design \( \mathcal{X}_l \) should satisfy the quasi-uniformity property discussed in Section 3.1. One way to satisfy both properties is first choose a quasi-uniform sequence \( \{z_i\}_{i=1}^{\infty} \) on the domain \( \Omega \), then construct the multi-level designs as \( \mathcal{X}_l = \{z_i\}_{i=1}^{nu}, \ l = 1, \ldots, L \). There are many ways of constructing such a quasi-uniform sequence; see, e.g., the low-dispersion sequences proposed in [47]. In our later implementation, we made use of a underlying Sobol’ sequence [35] for design construction, which appeared to yield good empirical performance in experiments.

We now describe the proposed stacking design algorithm in detail. The algorithm begins by selecting an initial fidelity level \( L = 1 \), then choosing an initial pilot design \( \mathcal{X}_0 \) of size \( n_0 \). Here, the initial sample size \( n_0 \) can be set as \( 10d \) as recommended in [23]. We then iterate the following steps:

1. Run the simulator at fidelity level \( L \) and observe \( f_L(x) \) at the pilot design \( \mathcal{X}_0 \). Estimate the MLGP parameters \( \{\Theta_l\}_{l=1}^{L} \) and \( \{\nu_l\}_{l=1}^{L} \) via maximum likelihood, and the RKHS norms \( \{|f_l - f_{l-1}|_{\mathcal{X}_0, (\Omega)}\}_{l=1}^{L} \) using the approach in Section 3.1.
2. Using these estimated parameters, compute the optimal sample sizes \( n_l \) via (3.6) and (3.10) for the current fidelity levels \( l = 1, \ldots, L \). With this, construct designs \( \mathcal{X}_l \) (with sample size \( n_l \)) to satisfy a nested structure, i.e., \( \mathcal{X}_0 \subseteq \mathcal{X}_L \subseteq \mathcal{X}_{L-1} \subseteq \cdots \subseteq \mathcal{X}_1 \). Run the simulators at these design points at their respective fidelity levels.

3. If the number of fidelity levels \( L \geq 3 \), estimate the rate parameter \( \alpha \) in (3.11) via regression (see Section 3.2). Using this estimate, test convergence via the stopping rule (3.14).

4. If convergence is not satisfied, iterate \( L \leftarrow L + 1 \) and repeat the above three steps. Otherwise, stop the sequential design and return the MLGP emulator (3.1).

Note that the computed sample sizes from Step 2 aim to control the emulation error \( |f_L(x) - \hat{f}_L(x)| \) (see Section 3.1), and the stopping rule in Step 3 aims to control the simulation error \( |f_\infty(x) - f_L(x)| \) (see Section 3.2). The workflow of this sequential design algorithm is visualized in Figure 2, and further details on the algorithm can be found in Supplementary Material S2.

While this stacking design algorithm ensures that the MLGP prediction error is bounded by \( \epsilon \), one may also wish to have a confidence interval which quantifies how uncertain our prediction is. This uncertainty again has two parts: (i) how uncertain the MLGP predictor \( f_L \) is from the simulated response surface \( f_L \), and (ii) how uncertain this simulated surface is from the exact solution \( f_\infty \). Confidence intervals for (i) can easily be constructed via the posterior predictive distribution in (2.4). One way to account uncertainty in (ii) is to integrate the upper bound of the numerical error, namely \( b(x) \) in (3.13). With this, we can construct a \( 100(1 - a)\% \) confidence intervals for \( f_\infty(x) \) as:

\[
\left( \sum_{l=1}^{L} \Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} z_l - q_a \sqrt{\sum_{l=1}^{L} \sigma_l^2 (\Phi_l(x, x) - \Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} \Phi_l(x, \mathcal{X}_l)^T) - b(x)}, \right.
\]

\[
\left. \sum_{l=1}^{L} \Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} z_l + q_a \sqrt{\sum_{l=1}^{L} \sigma_l^2 (\Phi_l(x, x) - \Phi_l(x, \mathcal{X}_l) \Phi_l^{-1} \Phi_l(x, \mathcal{X}_l)^T) + b(x)} \right),
\]

where \( q_a \) is the \( a \)-th quantile of the standard normal distribution.

For the practical choice of the desired prediction accuracy \( \epsilon \), one can begin with a large \( \epsilon \) to conduct the proposed stacking design, and if the prediction performance is not satisfactory (e.g., unsatisfactory predictions when comparing with validation simulations), the prediction accuracy can be subsequently improved by performing a “post” stacking design. More precisely, one can increase the precision by further selecting a smaller \( \epsilon \) and iterating the above steps of the algorithm starting from the fidelity level \( L \), at which the previous stacking design was terminated. This can be naturally done because the additional design points can be stacked on the previous stacking design.

4. Cost complexity theorem. With this in hand, we now investigate the computational complexity of the proposed stacking designs with the MLGP model. We show in the following theorem that, under regularity conditions, the MLGP can uniformly achieve the desired prediction error of \( \epsilon \) at a guaranteed rate for \( C_{tot} \), the total computational budget for training data simulation. Such a result can be viewed as an extension of cost complexity theorems in
Simulate $f_L$ on an initial pilot design $X_0$

Compute sample sizes $n_l$ via (3.6) and (3.10) and simulate $f_l$ on design $X_l$, for $l = 1, \ldots, L$

Test for error convergence via (3.14)

Is $L \geq 3$ and converged?

no

$L = L + 1$

yes

Return the fitted MLGP emulator (3.1)

Figure 2. Visualizing the sequential workflow for the proposed stacking design algorithm.

the multi-level Monte Carlo literature (see, e.g., [11]), which explore cost complexity rates required to ensure the precision of multi-level integral estimates. To our knowledge, such a result has yet to be explored for multi-level (or multi-fidelity) Gaussian process emulation.

Let $C_l$ denote the computational cost required for a single simulation run at fidelity level $l$, and let $C_{\text{tot}} = \sum_{l=1}^{L} n_l C_l$. Our cost complexity theorem is stated as follows:

Theorem 4.1. Suppose $\Omega$ is bounded and convex, with $\Phi_l$ taken as the Matérn kernel (2.5). Further suppose the smoothness parameters $\nu_l = \nu$ for each level $l$, with $2\nu$ a positive integer.

1. the simulation error $|f_{\infty}(x) - f_l(x)|$ is bounded as in (3.11),
2. the refinement function $(f_l - f_{l-1}) \in N_{\Phi_l}(\Omega)$ and the extended function $(f_l - f_{l-1}) \in H^{2\nu + d}(\mathbb{R}^d)$, where $H^m(\mathbb{R}^d)$ is a Sobolev space on $\mathbb{R}^d$, and $g \in N_{\Phi}(\Omega)$ is an extension of $g \in N_{\Phi}(\Omega)$ onto $N_{\Phi}(\mathbb{R}^d)$ (see [40] for further details),
3. the kernel length-scale parameters are bounded as $\|\Theta_l\|_2 < c_2$,
4. the designs $X_l$ are quasi-uniform, i.e., $h_X < c_3 n_l^{-1/d}$,
5. the computational cost $C_l$ is bounded as $C_l \leq c_4 \xi_l^{-\beta}$.

Assuming an error tolerance of $0 < \epsilon < e^{-1}$, there then exists choices of $L$ and $n_1, \ldots, n_L$ for which the MLGP emulator achieves the desired prediction bound

$$|f_{\infty}(x) - \hat{f}_L(x)| \leq \epsilon, \quad x \in \Omega,$$

with a total computational cost $C_{\text{tot}}$ bounded by

$$C_{\text{tot}} \leq \begin{cases} c_5 \epsilon^{-\frac{d}{\nu}}, & \frac{a}{\beta} > \frac{2\nu}{d}, \\ c_5 \epsilon^{-\frac{d}{\nu}} \log(\epsilon^{-1})^{1 + \frac{d}{\nu}}, & \frac{a}{\beta} = \frac{2\nu}{d}, \\ c_5 \epsilon^{-\frac{d}{\nu}} - 2^{\frac{d}{\nu} - \alpha} \log(\epsilon^{-1})^{1 + \frac{d}{\nu}}, & \frac{a}{\beta} < \frac{2\nu}{d}. \end{cases}$$

where $c_5$ is a positive constant.

The proof is given in Supplementary Material S3.
While this theorem is quite involved, it provides several novel and useful insights on the multi-fidelity design problem. For a given fidelity level \( l \), using the optimal allocation (3.6) and the simulation error bound (3.11) along with the conditions in Theorem 4.1, it follows that its optimal sample size \( n_l \) and its corresponding computational work \( n_l \xi_l^{-\beta} \) satisfies

\[
(4.2) \quad n_l \propto \xi_l \frac{(\alpha+2)\nu}{2(\nu+d)} \quad \text{and} \quad n_l \xi_l^{-\beta} \propto \xi_l \frac{\alpha d - 2 \beta \nu}{2(\nu+d)}, \quad l = 1, \ldots, L,
\]

where \( \xi_l \) is again the fidelity parameter for level \( l \). From this, a key factor for determining how much of the total budget \( C_{\text{tot}} \) to allocate to each fidelity is whether the numerator of the last term \( \alpha d - 2 \beta \nu > 0 \), or equivalently, the factor \( \alpha/\beta > 2 \nu/d \). When \( \alpha/\beta > 2 \nu/d \), one can see from (4.2) that much of the budget \( C_{\text{tot}} \) is expended on the levels with lower fidelities, i.e., with coarser mesh densities. Conversely, when \( \alpha/\beta < 2 \nu/d \), much of the budget will be allocated to levels with higher fidelities, i.e., with denser mesh densities.

One can further glean intuition on the terms \( \alpha/\beta \) and \( 2 \nu/d \) in this comparison. Recall that the parameters \( \alpha, \beta, \nu \) and \( d \) correspond to the rate parameter for simulator error convergence (see (3.11)), the rate of increase in computational cost as fidelity increases, the smoothness of the refinement function \( (f_l - f_{l-1}) \), and the number of input parameters, respectively. One can thus interpret the first fraction \( \alpha/\beta \) as the rate of simulator error reduction over the rate of computational cost increase as fidelity increases. Similarly, the second fraction \( 2 \nu/d \) can be interpreted as the rate of convergence for the underlying GP interpolator (see, e.g., [43]). Thus, when \( \alpha/\beta \) exceeds this rate of convergence for the GP (due to a combination of (i) and (ii)), the design procedure would shift more computational resources towards lower fidelity simulation runs, which is quite intuitive.

To further explore this idea, we compare next the cost complexity rate in Theorem 4.1 with the corresponding rate if our emulator were trained using only high-fidelity simulation data. Note that the fidelity level chosen for this latter high-fidelity emulator may be different from the high-fidelity level \( L \) for the MLGP emulator; to distinguish this, we will use fidelity level \( H \) with corresponding fidelity parameter \( \xi_H \). For this high-fidelity emulator, its predictor is given by the RKHS interpolator of \( f_H|\mathcal{X}_H \), i.e.,

\[
(4.3) \quad \hat{f}_H(x) = \Phi_H(x, \mathcal{X}_H)\Phi_H^{-1}\mathcal{Y}_H,
\]

where \( \mathcal{Y}_H := f_H|\mathcal{X}_H \) is the response vector simulated at fidelity level \( H \). The following corollary shows a similar cost complexity result for this high-fidelity GP emulator:

**Corollary 4.2.** Assume there exists positive constants \( c_1 \) and \( c_2 \) such that

1. there exist some \( \xi_H > 0 \) and \( 0 < \epsilon < 1 \) for which \((\epsilon/2)^{1+\frac{ad}{2}} \leq c_1 \xi_H^\alpha \leq \epsilon / 2 \),
2. the high-fidelity response surface \( f_H \in \mathcal{N}_{\Phi_H}(\Omega) \) and the extended function \( (f_H)_e \in H^{2\nu+d}(\mathbb{R}^d) \),
3. the kernel length-scale parameter is bounded as \( \|\Theta_H\|_2 < c_2 \).

Then there exists a sample size \( n_H \) for which the high-fidelity emulator (4.3) achieves the desired prediction bound

\[
|f_{\infty}(x) - \hat{f}_H(x)| \leq \epsilon, \quad x \in \Omega,
\]

with a total computational cost \( C_H \) bounded by

\[
(4.4) \quad C_H \leq c_h \epsilon^{-\frac{\beta}{\pi}} \frac{d}{\epsilon^\nu},
\]
where \( c_h \) is a positive constant.

By comparing the above rate with the complexity rate (4.1) for the multi-level GP (Theorem 4.1), one can gain illuminating insights on when multi-fidelity GP emulation improves upon standard high-fidelity GPs. Note that when \( \alpha/\beta < 2\nu/d \) (the same ratio compared earlier), the multi-level GP rate improves upon the high-fidelity GP rate, and conversely when \( \alpha/\beta \geq 2\nu/d \), the high-fidelity rate is quicker than the multi-level rate. Such a condition is intuitive and can be reasoned from the rate parameters \( \alpha \) and \( \beta \). For \( \alpha \), take the limiting setting of \( \alpha \to \infty \), such that the simulation error (3.11) decreases rapidly to zero as fidelity increases. In this setting, it is intuitive that a high-fidelity GP (which relies solely on such high-accuracy runs) would outperform the multi-fidelity GP; this is then affirmed by the fact that the condition \( \alpha/\beta \geq 2\nu/d \) is satisfied. For \( \beta \), take the limiting setting of \( \beta \to 0 \), such that the computational cost \( C_l \) grows slowly as fidelity increases. In this case, it makes sense that a high-fidelity GP (which would not be costly) would outperform the multi-fidelity GP given a fixed budget; this is again affirmed by the condition \( \alpha/\beta \geq 2\nu/d \). Similar conclusions also hold in reverse: when \( \alpha \to 0 \) or \( \beta \to \infty \), i.e., when the simulation error (3.11) decreases rapidly to zero or the cost \( C_l \) grows rapidly as fidelity increases, analogous reasoning can be used to explain why the multi-fidelity GP would be more preferable than the high-fidelity GP given a fixed cost budget. In this view, Theorem 4.1 provides a novel perspective on when multi-fidelity modeling improves upon high-fidelity modeling for GP emulation.

It should be noted that, in the above comparison, it is assumed that one knows the high-fidelity fidelity parameter \( \xi_H \) such that Condition 1 in Corollary 4.2 is satisfied. For practical implementation, such a fidelity parameter is typically not known, and a misspecification of this \( \xi_H \) can lead to a worse cost complexity rate than what is guaranteed by Corollary 4.2 for the high-fidelity GP. The proposed stacking design gets around this issue of “fidelity misspecification”, by employing a sequential sampling approach for determining the number of levels \( L \) and corresponding sample sizes \( n_1, \cdots, n_L \) to achieve the desired error tolerance.

5. Numerical Experiments. We now investigate a suite of numerical experiments to examine the proposed stacking designs, in particular, its predictive performance and its ability to achieve a desired error tolerance with confidence. Section 5.1 explores a synthetic example, Section 5.2 investigates an application to Poisson’s equation, and Section 5.3 considers an application for thermal stress analysis of a jet engine turbine blade. The latter two problems involve partial differential equation (PDE) systems which are numerically solved via finite element modeling. These experiments are all initialized with an initial design \( X_0 \) of size \( n_0 = 5d \). All experiments are performed on a MacBook Pro laptop with Apple M1 Max Chip and 32Gb of RAM.

5.1. Multi-fidelity Currin function. We first consider the following two-dimensional multi-fidelity Currin function:

\[
\begin{align*}
    f_l(x_1, x_2) &= f_\infty(x_1, x_2) + \xi^a_l \exp(-1.4x_1) \cos(3.5\pi x_2).
\end{align*}
\]
Here, $f_\infty(x_1, x_2)$ is the Currin test function [5] which we take to be our limiting highest-fidelity setting:

$$f_\infty(x_1, x_2) = \left[ 1 - \exp\left( -\frac{1}{2x_2} \right) \right] \frac{2300x_1^3 + 1900x_2^3 + 2092x_1 + 60}{100x_1^2 + 500x_2^2 + 4x_1 + 20}, \quad (x_1, x_2) \in [0, 1]^2 = \Omega.$$ 

The remaining term in (5.1) is the discrepancy term, which converges to zero as fidelity parameter $\xi_l$ increases and makes (5.1) satisfy the inequality of (3.11) because $|\exp(-1.4x_1) \cos(3.5\pi x_2)|$ is bounded by $c_1 = 1$. In the following, we set $\alpha = 1$ and $\xi_l = \xi_0 T^{-l} = 16 \times 2^{-l}$, and set the computational cost to be $C_l = 4^l$. We assume that $\alpha$ is unknown which needs to be estimated. Figure 3 shows the synthetic functions $f_l(x_1, x_2)$ for fidelity levels $l = 1, 2, 3$ and the limiting function $f_\infty(x_1, x_2)$. With this, we then applied the stacking design algorithm from Section 3.3, with the desired prediction accuracy is set as $\epsilon = 1$ in $L_2$ norm.

The stacking design begins with $L = 1$, which requires $n_1 = 23$ design points on the lowest fidelity simulator $f_1$ (left panel of Figure 4) to ensure that the estimated emulation error bound (3.9) of $\|f_1 - \hat{f}_l\|_{L_2(\Omega)}$ is smaller than $\epsilon/2 = 0.5$; this is summarized in the $L = 1$ column in Table 1. In the next step with $L = 2$, we then add an additional 39 design points for the lower-fidelity simulator $f_1$, yielding a total of $n_1 = 62$ runs on $f_1$. We then add $n_2 = 34$ design points on a higher-fidelity simulator $f_2$ (i.e., fidelity level $l = 2$), which is then “stacked” on top of the lower-fidelity design (second panel from the left of Figure 4). With the designs conducted at these two fidelity levels, the estimated emulation error bound $\|f_2 - \hat{f}_l\|_{L_2(\Omega)}$ comes to 0.497, which is again less than $\epsilon/2 = 0.5$. We then repeat this iteratively for increasing fidelity levels $L = 3$ and $L = 4$, after which the stopping rule (3.14) is satisfied and the procedure is terminated. Figure 4 visualizes the experimental designs and corresponding samples sizes at each step.

To evaluate the simulation error bound in the stopping rule (3.14), the rate parameter $\alpha$ needs to be estimated from data; this can be done via (3.12) when $L \geq 3$. Figure 5 illustrates this estimation using a fitted log-transformed linear regression model (red lines), with estimates of $\alpha$ reported in Table 1. With the estimate of $\alpha$ at $L = 3$, the simulation error bound (3.14) gives 0.681, which is greater than $\epsilon/2$ and thus the sequential design continues. With the
Figure 4. (Top) The proposed stacking designs at \( L = 4 \) fidelity levels, over four sequential design stages (from left to right). (Bottom) The corresponding sample sizes at the \( L = 4 \) fidelity levels, over four sequential design stages (from left to right).

| \( L = 1 \) | \( L = 2 \) | \( L = 3 \) | \( L = 4 \) |
|-------------|-------------|-------------|-------------|
| Fidelity parameter | \( \xi_1 = 8 \) | \( \xi_2 = 4 \) | \( \xi_3 = 2 \) | \( \xi_4 = 1 \) |
| Cost per run | \( C_1 = 4 \) | \( C_2 = 16 \) | \( C_3 = 64 \) | \( C_4 = 256 \) |
| Bound of \( \| f_{\infty} - f_L \|_{L_2(\Omega)} \) | NA | NA | 0.681 | 0.400 |
| (\( \hat{\alpha} = 1.12 \)) | (\( \hat{\alpha} = 0.96 \)) |
| Bound of \( \| f_L - \hat{f}_L \|_{L_2(\Omega)} \) | 0.483 | 0.497 | 0.490 | 0.453 |

Table 1

The estimated simulation and emulation error bounds (see (3.14) and (3.9), respectively) at each design stage for the multi-fidelity Currin experiment, with estimated rate parameter \( \hat{\alpha} \) at stages \( L = 3 \) and \( L = 4 \). Bolded numbers indicate the error is less than \( \epsilon/2 \), where \( \epsilon = 1 \) is the desired error tolerance.

The estimate of \( \alpha \) at \( L = 4 \), the simulation error estimate is less than \( \epsilon/2 = 0.5 \), thus the stopping rule is satisfied and the design procedure stops. Table 1 shows the estimated upper bounds for simulation and emulation errors, both of which need to be smaller than \( \epsilon/2 = 0.5 \) for the procedure to stop. The \( L_2 \)-error of the final MLGP emulator (estimated via Monte Carlo integration) is \( \| f_{\infty} - \hat{f}_L \|_{L_2(\Omega)} = 0.55 \), which is indeed smaller than the desired prediction accuracy of \( \epsilon = 1 \). This shows that the proposed stacking designs, by increasing fidelity levels and stacking design points in a sequential fashion, can indeed satisfy the desired error bound with confidence.
Finally, we explore the performance of stacking designs for different choices of error tolerance $\epsilon$, using both $L_2$ and $L_\infty$ norms. Figure 6 visualizes the sample sizes (at each fidelity level) and the corresponding errors of the final MLGP emulator. We see that, for different $\epsilon$ and different norms, the proposed stacking designs can consistently yield prediction errors which are smaller than the desired error tolerance $\epsilon$, which is as desired.

5.2. Poisson’s equation. Next, we explore the performance of stacking designs for emulating an elliptical PDE system. The system of interest is modeled using Poisson’s equation on a square membrane [8], which has broad applicability in electrostatics and fluid mechanics. This can be represented by the PDE:

$$\Delta u = (x^2 - 2\pi^2)e^{xz_1}\sin(\pi z_1)\sin(\pi z_2) + 2x\pi e^{xz_1}\cos(\pi z_1)\sin(\pi z_2), \quad (z_1, z_2) \in D,$$

where $u(z_1, z_2)$ is the solution of interest, $\Delta = \partial^2/\partial z_1^2 + \partial^2/\partial z_2^2$ is the Laplace operator, $D \in [0, 1] \times [0, 1]$, and $x \in \Omega = [-1, 1]$. One then imposes the Dirichlet boundary condition...
$u = 0$ on the boundary $\partial D$. Following [41], FEM is used to solve this system numerically. In our implementation, we make use of the Partial Differential Equation Toolbox of [26] to create the geometry and mesh. In the toolbox, one can specify the mesh size for the numerical solver; Figure 7 visualizes the numerical solutions of (5.2) with three different choices of mesh sizes.

Here, the response of interest is taken as the integral of the solution $f_\infty(x) = \int u(z_1, z_2)dz_1dz_2$. It can be shown that this solution has the analytical form [41]:

$$f_\infty(x) = \frac{2(e^x + 1)}{x^2 + \pi^2}.$$

Of course, in practical problems, one does not typically have such closed-form solutions; this framework was chosen to allow for easy validation of the fitted emulator model. For the stacking designs, we again define a geometric sequence of fidelity parameters (here, mesh sizes) $\xi_l = \xi_0 T^{-l} = 0.4 \times 2^{-l}, l = 1, 2, \ldots$. We then set a desired prediction accuracy of $\epsilon = 0.05$ for the $L_\infty$-norm.

Figure 8 shows the fitted MLGP predictor and uncertainty bands (upper panels), with its corresponding sample sizes at each fidelity level (bottom panels) at each step of the stacking design process. Table 2 shows the estimated emulation and simulation error bounds. In the first step with $L = 1$, the lowest fidelity simulation (with mesh size 0.2) is run with a design of size $n_1 = 5$. From the left panels in Figure 8, the resulting fitted MLGP model $\hat{f}_1$ appears to be biased with very wide confidence bands. In the third step ($L = 3$), additional design points are stacked on fidelity levels 2 and 3 ($n_1 = 5, n_2 = 5, n_3 = 5$), and the simulation error rate parameter $\alpha$ is then estimated (see Figure 9). With this estimated parameter, the estimated simulation error bound (3.14) evaluates to 0.047 (see Table 2), which is being greater than $\epsilon/2 = 0.025$. The process thus continues until the fifth step ($L = 5$), in which both the simulation and emulation error bounds become smaller than $\epsilon/2$. From the right panels in Figure 8, the resulting fitted emulator $\hat{f}_5$ appears to yield an accurate prediction with narrow confidence bands. The $L_\infty$-error of this final multi-fidelity emulator (estimated via grid search optimization) is $\|f_\infty - \hat{f}_5\|_{L_\infty(\Omega)} = 0.016$, which is smaller than the desired prediction accuracy $\epsilon = 0.05$. This again shows that the proposed stacking designs, by iteratively increasing fidelity levels and stacking design runs, can yield the desired error tolerance with confidence.
Figure 8. Visualizing the stacking design procedure for the Poisson’s equation experiment. (Top) The stacking design points (dots) and the fitted MLGP predictor with pointwise 95% confidence band (gray shaded region) over five sequential design stages (from left to right). (Bottom) The corresponding sample sizes at the $L = 4$ fidelity levels, over five sequential design stages (from left to right).

| $L$  | $\xi_1$ | $\xi_2$ | $\xi_3$ | $\xi_4$ | $\xi_5$ |
|------|--------|--------|--------|--------|--------|
| 1    | 0.2    | 0.1    | 0.05   | 0.025  | 0.0125 |
| 2    | 0.18   | 0.19   | 0.23   | 0.27   | 0.55   |

Bound of $\|f_\infty - f_L\|_{L_\infty(\Omega)}$ NA NA 0.047 0.030 0.008

Bound of $\|f_\infty - \hat{f}_L\|_{L_\infty(\Omega)}$ 0.009 0.010 0.011 0.011 0.011

Table 2

The estimated simulation and emulation error bounds (see (3.14) and (3.9), respectively) at each design stage for the Poisson’s equation experiment, with estimated rate parameter $\hat{\alpha}$ at stages $L = 3$ and $L = 4$. Bolded numbers indicate the error is less than $\epsilon/2$, where $\epsilon = 0.05$ is the desired error tolerance.

As before, we further explore the stacking designs for this problem with different error tolerances $\epsilon$ using both $L_2$ and $L_\infty$ norms. Figure 10 shows the sample sizes (at each fidelity level) and the corresponding errors of the final MLGP emulator. We see again that the proposed designs can indeed consistently satisfy the desired error tolerance $\epsilon$ with confidence. It is worth noting that, in this problem, a majority of the computational budget is expended on higher fidelity runs (i.e., with denser mesh densities), since the sample sizes are equally allocated over each fidelity level (see Figure 10). This is not too surprising: the fitted function is quite smooth ($\nu = 3.5$), and with estimated rate parameters $\hat{\alpha} \approx 1$ and $\hat{\beta} \approx 0.37$, the condition $\alpha/\beta < 2\nu/d$ can be shown to be satisfied (see earlier discussion of this condition in Section 4 and the cost complexity theorem).
5.3. Thermal Stress Analysis of Jet Engine Turbine Blade. Finally, we investigate the performance of the proposed designs on a thermal stress analysis application for a jet turbine engine blade in steady-state operating condition. Here, the turbine is a component of the jet engine, composed of a radial array of blades typically made from nickel alloys that resist extremely high temperatures. To avoid mechanical failure and friction between the tip of the blade and the turbine casing, it is crucial that the blade design can withstand stress and deformations. See [44] and [4] for more details. We thus wish to study here the effect of thermal stress and pressure of the surrounding gases on turbine blades. As before, this problem can be analyzed as a static structural model, which can be numerically solved using finite element modeling. The $d = 2$ input variables are the pressure load on the pressure ($x_1$) and suction ($x_2$) sides of the blade, both of which range from 0.25 to 0.75 MPa, i.e., $x_1, x_2 \in \Omega = [0.25, 0.75]^2$. The response of interest is taken as the integral of the solution over the thermal stress profile. FEM simulations are performed using the Partial Differential Equation Toolbox in MATLAB [26]. Figure 11 visualizes the blade structure and the simulated thermal stress profiles at three choices of mesh sizes.

For stacking designs, we make use of a geometric sequence of fidelity parameters (here,
Figure 11. Visualizing the FEM solutions for three choices of mesh sizes in the turbine blade application.

| Mesh size | $L = 1$ | $L = 2$ | $L = 3$ | $L = 4$ |
|-----------|---------|---------|---------|---------|
| $\xi_1$   | 0.05    | 0.025   | 0.0125  | 0.00625 |
| $\xi_2$   | 0.025   | 1.03    | 2.28    | 12.58   |
| $\xi_3$   |         |         |         |         |
| $\xi_4$   |         |         |         |         |

Table 3

The estimated simulation and emulation error bounds (see (3.14) and (3.9), respectively) at each design stage for the turbine blade application, with estimated rate parameter $\hat{\alpha}$ at stages $L = 3$ and $L = 4$. Bolded numbers indicate the error is less than $\epsilon/2$, where $\epsilon = 5$ is the desired error tolerance.

mesh sizes) $\xi_l = \xi_0 T^{-l} = 0.1 \times 2^{-l}, l = 1, 2, \ldots$. The desired prediction accuracy is then set to $\epsilon = 5$ in $L_2$-norm. Figure 1 shows the proposed stacking designs over each iteration, Table 3 summarizes the corresponding emulation and simulation error bounds, and Figure 12 shows the simulation discrepancy decay along with the estimates of $\alpha$. Here, we see that the MLGP requires $L = 4$ iterations (resulting in $L = 4$ fidelity levels for the final emulator) to achieve the desired prediction accuracy. Unlike in Section 5.2, the true function $f_\infty(x)$ cannot be expressed in closed form; we thus perform validation runs at 20 uniformly sampled input settings with a small mesh size of $\xi_5 = 3.125 \times 10^{-3}$. Figure 13 visualizes the final MLGP predictor $\hat{f}_L(x_1, x_2)$ as in (3.1) with the out-of-sample test points (red points), as well as the widths of 95% confidence interval over the input space. We see that the predicted response surface quite closely mimics the test data, which is as desired. This is confirmed by the empirical $L_2$-norm of prediction error on the test data (2.01), which is smaller than the desired error tolerance of $\epsilon = 5$. This again shows that the proposed stacking designs can indeed achieve the desired prediction accuracy with confidence via iterative multi-fidelity modeling.
Figure 12. Plotting the logarithm of the absolute value of the refinement (i.e., $\log|f_l(x) - f_{l-1}(x)|$) as a function of $\log(T^{-1})$ in the turbine blade application. The red dashed line shows the line of best fit, with its slope indicating the estimate of $\alpha$.

Figure 13. (Left) Visualizing the fitted MLGP predictor with the test design points in red. (Right) Visualizing the pointwise 95% confidence interval widths over the design space.

6. Concluding Remarks. In this work, we proposed a novel stacking design approach for multi-fidelity GP modeling, which provides a sequential approach for designing multi-fidelity runs to achieve a desired prediction error $\epsilon > 0$ with confidence. This addresses a key limitation of existing design methods, and allows for confident and cost-efficient predictive computing for a broad range of scientific and engineering problems. We then proved a cost complexity theorem which, under the employed multi-level GP emulator, establishes a bound on computational cost (of training data simulation) needed to ensure a desired prediction error tolerance of $\epsilon$. A corollary then provides new insight on when the presented multi-fidelity GP emulator yields improved predictive performance over a single-fidelity GP model. A suite of numerical experiments, including an application to jet turbine blade analysis, shows that the proposed method can efficiently and accurately emulate multi-fidelity computer experiments with confidence.
Supplemental Materials Additional supporting materials can be found in Supplemental Materials, including the detailed proofs of Proposition 3.1, Theorem 4.1, and Corollary 4.2, the detailed algorithm for Section 3.3, and the R code for reproducing the results in Section 5.

REFERENCES

[1] S. C. Brenner and L. R. Scott, The Mathematical Theory of Finite Element Methods (Third Edition), New York: Springer, 2007.
[2] R. E. Caplisch, Monte Carlo and quasi-Monte Carlo methods, Acta Numerica, 7 (1998), pp. 1–49.
[3] S. Cao, Y. Chen, J. Coleman, J. Mulligan, P. Jacobs, R. Soltz, A. Angerami, R. Arora, S. Bass, L. Cunqueiro, et al., Determining the jet transport coefficient $\hat{q}$ from inclusive hadron suppression measurements using Bayesian parameter estimation, Physical Review C, 104 (2021), p. 024905.
[4] T. J. Carter, Common failures in gas turbine blades, Engineering Failure Analysis, 12 (2005), pp. 237–247.
[5] C. Curran, T. Mitchell, M. Morris, and D. Ylvisaker, A Bayesian approach to the design and analysis of computer experiments, tech. report, Oak Ridge National Lab., TN (USA), 1988.
[6] C. Curran, T. Mitchell, M. Morris, and D. Ylvisaker, Bayesian prediction of deterministic functions, with applications to the design and analysis of computer experiments, Journal of the American Statistical Association, 86 (1991), pp. 953–963.
[7] A. Eshara and S. Guillias, An adaptive strategy for sequential designs of multilevel computer experiments, arXiv:2104.02037, (2021).
[8] L. C. Evans, Partial Differential Equations (Second Edition), vol. 19, American Mathematical Society, 2010.
[9] D. Everett, W. Ke, J.-F. Paquet, G. Vujanovic, S. Bass, L. Du, C. Gale, M. Heffernan, U. Heinz, D. Liyanage, et al., Multisystem Bayesian constraints on the transport coefficients of QCD matter, Physical Review C, 103 (2021), p. 054904.
[10] K.-T. Fang and Y. Wang, Number-Theoretic Methods in Statistics, vol. 51, CRC Press, 1993.
[11] M. B. Giles, Multilevel monte carlo path simulation, Operations research, 56 (2008), pp. 607–617.
[12] M. B. Giles, Multilevel monte carlo methods, Acta Numerica, 24 (2015), pp. 259–328.
[13] R. B. Gramacy, Surrogates: Gaussian Process Modeling, Design, and Optimization for the Applied Sciences, Chapman and Hall/CRC, 2020.
[14] B. Haaland and P. Z. G. Qian, Accurate emulators for large-scale computer experiments, The Annals of Statistics, 39 (2011), pp. 2974–3002.
[15] X. He, R. Tuo, and C. J. Wu, Optimization of multi-fidelity computer experiments via the EQIE criterion, Technometrics, 59 (2017), pp. 58–68.
[16] W. H. Hundsdorfer and J. G. Verwer, Numerical Solution of Time-dependent Advection-diffusion-reaction Equations, vol. 33, Springer, 2003.
[17] Y. Ji, S. Mak, D. Soeder, J.-F. Paquet, and S. A. Bass, A graphical multi-fidelity Gaussian process model, with application to emulation of expensive computer simulations, 2022, https://arxiv.org/abs/2108.00306.
[18] Y. Ji, H. S. Yuchi, D. Soeder, J.-F. Paquet, S. A. Bass, V. R. Joseph, C. Wu, and S. Mak, Multi-stage multi-fidelity Gaussian process modeling, with application to heavy-ion collisions, arXiv preprint arXiv:2209.13748, (2022).
[19] M. C. Kennedy and A. O’Hagan, Predicting the output from a complex computer code when fast approximations are available, Biometrika, 87 (2000), pp. 1–13.
[20] L. Le Gratiet, Bayesian analysis of hierarchical multifidelity codes, SIAM/ASA Journal on Uncertainty Quantification, 1 (2013), pp. 244–269.
[21] L. Le Gratiet and C. Cannamela, Cokriging-based sequential design strategies using fast cross-validation techniques for multi-fidelity computer codes, Technometrics, 57 (2015), pp. 418–427.
[22] L. Le Gratiet and J. Garnier, Recursive co-kriging model for design of computer experiments with multiple levels of fidelity, International Journal for Uncertainty Quantification, 4 (2014).
[23] J. L. Loeppky, J. Sacks, and W. J. Welch, Choosing the sample size of a computer experiment: A practical guide, Technometrics, 51 (2009), pp. 366–376.
[24] S. Mak and V. R. Joseph, Minimax and minimax projection designs using clustering, Journal of Computational and Graphical Statistics, 27 (2018), pp. 166–178.
[25] S. Mak, C.-L. Sung, X. Wang, S.-T. Yeh, Y.-H. Chang, V. R. Joseph, V. Yang, and C. F. J. Wu, An efficient surrogate model for emulation and physics extraction of large eddy simulations, Journal of the American Statistical Association, 113 (2018), pp. 1443–1456.
[26] MATLAB, MATLAB version 9.11.0.1769968 (R2021b), The Mathworks, Inc., Natick, Massachusetts, 2021.
[27] S. Müller, Komplexität und Stabilität von kernbasierten Rekonstruktionsmethoden, PhD thesis, Niedersächsische Staats-und Universitätsbibliothek Göttingen, 2009.
[28] S. Myren and E. Lawrence, A comparison of Gaussian processes and neural networks for computer model emulation and calibration, Statistical Analysis and Data Mining, 14 (2021), pp. 606–623.
[29] P. Perdikaris, M. Raissi, A. Damianou, N. D. Lawrence, and G. E. Karniadakis, Nonlinear information fusion algorithms for data-efficient multi-fidelity modelling, Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 473 (2017), p. 20160751.
[30] S. Pettit, J. Bect, P. Feliot, and E. Vazquez, Gaussian process interpolation: the choice of the family of models is more important than that of the selection criterion, arXiv preprint arXiv:2107.06006, (2021).
[31] P. Z. G. Qian and C. F. J. Wu, Bayesian hierarchical modeling for integrating low-accuracy and high-accuracy experiments, Technometrics, 50 (2008), pp. 192–204.
[32] C. E. Rasmussen and C. K. Williams, Gaussian Processes for Machine Learning, MIT press Cambridge, MA, 2006.
[33] J. Sacks, W. J. Welch, T. J. Mitchell, and H. P. Wynn, Design and analysis of computer experiments, Statistical Science, 4 (1989), pp. 409–423.
[34] T. J. Santner, B. J. Williams, and W. I. Notz, The Design and Analysis of Computer Experiments (Second Edition), Springer New York, 2018.
[35] I. M. Sobol’, On the distribution of points in a cube and the approximate evaluation of integrals, Zhurnal Vychislitel’noi Matematiki i Matematicheskoi Fiziki, 7 (1967), pp. 784–802.
[36] M. L. Stein, Interpolation of Spatial Data: Some Theory for Kriging, Springer Science & Business Media, 2012.
[37] J. A. Templeton, M. L. Blaylock, S. P. Domino, J. C. Hewson, P. R. Kumar, J. Ling, H. N. Najm, A. Ruiz, C. Safta, K. Sargsyan, et al., Calibration and forward uncertainty propagation for large-eddy simulations of engineering flows, tech. report, Sandia National Lab.(SNL-CA), Livermore, CA (United States); Sandia National Lab.(SNL-NM), Albuquerque, NM (United States), 2015.
[38] R. K. Tripathy and I. Bilionis, Deep UQ: Learning deep neural network surrogate models for high dimensional uncertainty quantification, Journal of Computational Physics, 375 (2018), pp. 565–588.
[39] R. Tuo and W. Wang, Kriging prediction with isotropic matern correlations: Robustness and experimental designs., Journal of Machine Learning Research, 21 (2020), pp. 1–38.
[40] R. Tuo, Y. Wang, and C. F. J. Wu, On the improved rates of convergence for Matérn-type kernel ridge regression with application to calibration of computer models, SIAM/ASA Journal on Uncertainty Quantification, 8 (2020), pp. 1522–1547.
[41] R. Tuo, C. F. J. Wu, and D. Yu, Surrogate modeling of computer experiments with different mesh densities, Technometrics, 56 (2014), pp. 372–380.
[42] W. Wang, R. Tuo, and C. F. Jeff Wu, On prediction properties of kriging: Uniform error bounds and robustness, Journal of the American Statistical Association, 115 (2020), pp. 920–930.
[43] H. Wendland, Scattered Data Approximation, vol. 17, Cambridge university press, 2004.
[44] L. M. Wright and J.-C. Han, Enhanced internal cooling of turbine blades and vanes, The Gas Turbine Handbook, 4 (2006), pp. 1–5.
[45] G. Wynne, F.-X. Briol, and M. Girolami, Convergence guarantees for Gaussian process means with misspecified likelihoods and smoothness, Journal of Machine Learning Research, 22 (2021), pp. 1–40.
[46] D. Xiu, Numerical methods for stochastic computations, in Numerical Methods for Stochastic Computations, Princeton university press, 2010.
[47] S. Yakowitz, P. L’ecuyer, and F. Vazquez-Abad, Global stochastic optimization with low-dispersion point sets, Operations Research, 48 (2000), pp. 939–950.
Supplementary Materials for “Stacking designs: designing multi-fidelity computer experiments with confidence”

**S1. Proof of Proposition 3.1.** Denote $P_l(x) = \Phi_l(x, X_l) \Phi_l^{-1} z_l$, which is the reproducing kernel Hilbert space (RKHS) interpolator of $(f_l - f_{l-1})|_{X_l}$ using kernel $\Phi_l$. Since $f_L = \sum_{l=1}^L (f_l - f_{l-1})$ and $\hat{f}_L = \sum_{l=1}^L P_l$, it follows that

$$|f_L(x) - \hat{f}_L(x)| = \left| \sum_{l=1}^L (f_l(x) - f_{l-1}(x)) - \sum_{l=1}^L P_l(x) \right|$$

$$= \left| \sum_{l=1}^L [(f_l(x) - f_{l-1}(x)) - P_l(x)] \right|$$

$$\leq \sum_{l=1}^L |(f_l(x) - f_{l-1}(x)) - P_l(x)|,$$  

(S1.1) where the last inequality follows the triangle inequality. Following Theorem 11.11 of [43] and Theorem 5.1 of [14], it follows that

$$|(f_l(x) - f_{l-1}(x)) - P_l(x)| \leq c_{\phi_{\nu_l}} \|\Theta_l\|_2^{\nu_l} h_{X_l}^{\nu_l} \|f_l - f_{l-1}\|_{N_{\Phi_l}(\Omega)}.$$

Define $c_0 = \max_{l=1,\ldots,L} c_{\phi_{\nu_l}}$. Then, combining with (S1.1), it concludes the proof.

**S2. Algorithm for MLGP emulator with stacking design.**

**Require:** $\epsilon > 0$

**Ensure:** $\|f_\infty - \hat{f}_L\| < \epsilon$

1: Set an initial sample $X_0$ of size $n_0$. $\triangleright n_0 \approx 5d \sim 10d$ is recommended

2: $L \leftarrow 1$

3: repeat

4: Evaluate $f_L(x)$ on initial design $X_0$

5: Estimate parameters $\Theta_l$ and $\nu_l$ and RKHS norm $\|f_l - f_{l-1}\|_{N_{\Phi_l}(\Omega)}$

6: Set sample sizes $n_l$ via (3.6) and (3.10)

7: Construct design $X_l$ of size $n_l$ satisfying $X_0 \subseteq X_L \subseteq X_{L-1} \subseteq \cdots \subseteq X_1$

8: Evaluate $f_l(x)$ on extra samples at each level as needed for new $X_l$

9: if $L \geq 3$ then

10: Estimate rate parameter $\alpha$ via linear regression with a log-transformation

11: Test for error convergence via (3.14)

12: else

13: $L \leftarrow L + 1$

14: end if

15: until converged via (3.14)

16: return MLGP emulator via (3.1)

**S3. Proof of Theorem 4.1.** We start by choosing $L$ to be

$$L = \left\lceil \frac{\log(2c_1\xi_0^\alpha \epsilon^{-1})}{\alpha \log T} \right\rceil$$  

(S3.1)
To bound the computational cost $C_{\alpha d}$, thus, by Conditions 4, 5, the equations (S3.3) and (S3.5), we have
\begin{equation}
|f_{\infty}(x) - f_L(x)| \leq c_1 \xi_1^\alpha \leq \frac{1}{2} \epsilon,
\end{equation}
and hence, by Condition 1,
\begin{equation}
|f_{\infty}(x) - f_L(x)| \leq c_1 \xi_1^\alpha \leq \frac{1}{2} \epsilon.
\end{equation}
By Theorem 2.2 in [40], Condition 3 implies that there exists $v_l \in L_2(\Omega)$, such that $f_l(x) - f_{l-1}(x) = \int_\Omega \Phi_l(x - y) v_l(y) dy$, and $\bar{v} := \sup_{l \in \mathbb{N}^+} ||v_l||_{L_2(\Omega)} < +\infty$. Thus, it follows that
\begin{equation}
\|f_l - f_{l-1}\|_{H^s(\Omega)} = (f_l - f_{l-1}, f_l - f_{l-1})_{H^s(\Omega)}
= (f_l - f_{l-1}, v_l)_{L_2(\Omega)}
\leq \|f_l - f_{l-1}\|_{L_2(\Omega)} \|v_l\|_{L_2(\Omega)}
\leq \bar{v} (\|f_l\|_{L_2(\Omega)} + \|f_l - f_{l-1}\|_{L_2(\Omega)})
\leq c_1 \bar{v} \text{Vol}(\Omega) (\xi_1^\alpha + \xi_1^\beta) \leq c_1 \bar{v} \text{Vol}(\Omega) (1 + T^\alpha) \xi_1^\alpha,
\end{equation}
where Vol($\Omega$) is the volume of $\Omega$. Then, combining (S3.4) and Conditions 4 and 5 with Theorem 3.1, it follows that
\begin{equation}
|f_L(x) - \hat{f}_L(x)| \leq c_0 \sum_{l=1}^{L} \|\Theta_l\|_{H^s(\Omega)} \|f_l - f_{l-1}\|_{H^s(\Omega)}
\leq c_0 c_1^{1/2} c_2^{\nu} c_3^{\beta} \bar{v}^{1/2} \text{Vol}(\Omega)^{1/2} (1 + T^\alpha)^{1/2} \sum_{l=1}^{L} n_l^{-\frac{\beta}{2}} \xi_l^\alpha/2.
\end{equation}
Thus, by Conditions 4, 5, the equations (S3.3) and (S3.5), we have
\begin{equation}
|f_{\infty}(x) - \hat{f}_L(x)| \leq |f_{\infty}(x) - f_L(x)| + |f_L(x) - \hat{f}_L(x)|
\leq \frac{\epsilon}{2} + c_0 c_1^{1/2} c_2^{\nu} c_3^{\beta} \bar{v}^{1/2} \text{Vol}(\Omega)^{1/2} (1 + T^\alpha)^{1/2} \sum_{l=1}^{L} n_l^{-\frac{\beta}{2}} \xi_l^\alpha/2.
\end{equation}
The second term will be discussed separately given $\alpha d = 2\beta \nu, \alpha d > 2\beta \nu$ and $\alpha d < 2\beta \nu$. For notational simplicity, we let $c_0 = c_0 c_1^{1/2} c_2^{\nu} c_3^{\beta} \bar{v}^{1/2} \text{Vol}(\Omega)^{1/2} (1 + T^\alpha)^{1/2}$.

If $\alpha d = 2\beta \nu$, we set $n_l = \left(2L c_0^{-1} \xi_l^\beta \right)^{\frac{d}{\beta}}$ so that
\begin{equation}
|f_{\infty}(x) - \hat{f}_L(x)| \leq \frac{\epsilon}{2} + c_6 \sum_{l=1}^{L} n_l^{-\frac{\beta}{2}} \xi_l^{\alpha/2} \leq \frac{\epsilon}{2} + c_6 \frac{\epsilon}{2L c_0} L \xi_l^\alpha \leq \frac{\epsilon}{2} + \frac{\epsilon}{2} \leq \epsilon.
\end{equation}
To bound the computational cost $C_{\text{tot}}$, since the upper bound for $n_l$ is given by
\begin{equation}
n_l \leq \left(2L c_0^{-1} \xi_l^\beta \right)^{\frac{d}{\beta}} + 1,
\end{equation}
the computational cost is bounded by

\[
C_{\text{tot}} \leq c_4 \sum_{l=1}^{L} n_l \xi_l^{-\beta} \leq c_4 \left( (2c_6) \frac{d}{\nu} \mu L \nu \sum_{l=1}^{L} \xi_l^{-\beta} + \sum_{l=1}^{L} \xi_l^{-\beta} \right)
\]

(S3.6)

\[
\leq c_4 \left( (2c_6) \frac{d}{\nu} \mu L^{1+\frac{d}{\nu}} + \sum_{l=1}^{L} \xi_l^{-\beta} \right).
\]

By (S3.1), the upper bound on \( L \) is given by

\[
L \leq \frac{\log \epsilon^{-1}}{\alpha \log T} + \frac{\log(2c_1 \xi_0^\alpha)}{\alpha \log T} + 1.
\]

Given that \( 1 < \log \epsilon^{-1} \) for \( \epsilon < e^{-1} \), it follows that

(S3.7)

\[
L \leq c_7 \log \epsilon^{-1},
\]

where

\[
c_7 = \frac{1}{\alpha \log T} + \max \left( 0, \frac{\log(2c_1 \xi_0^\alpha)}{\alpha \log T} \right) + 1.
\]

Moreover, since \( \epsilon^{-1/\alpha} \leq \epsilon^{-\frac{d}{\nu}} \alpha \geq \frac{\beta \nu}{\alpha} \) and \( \epsilon < e^{-1} \), by (S3.2) it follows

(S3.8)

\[
\xi_L^{-1} < T \left( \frac{\epsilon}{2e_1} \right)^{-1/\alpha} l \beta \nu 1/\alpha \epsilon^{-\frac{d}{\nu}}.
\]

Then, by the standard result for a geometric series and the inequality in (S3.8),

\[
\sum_{l=1}^{L} \xi_l^{-\beta} = \xi_L^{-\beta} \sum_{l=1}^{L} (T^{-\beta})^{l-1-L} < \xi_L^{-\beta} (1 - T^{-\beta})^{-1}
\]

(S3.9)

\[
< 2^{\beta/\alpha} c_7^{\beta/\alpha} \frac{T^\beta}{1 - T^{-\beta}} \epsilon^{-\frac{d}{\nu}}.
\]

Thus, combining (S3.6), (S3.7), and (S3.9), and by the fact that \( 1 < \log \epsilon^{-1} \) for \( \epsilon < e^{-1} \), it follows that

\[
C_{\text{tot}} \leq c_5 \epsilon^{-\frac{d}{\nu}} \log(\epsilon^{-1})^{1+\frac{d}{\nu}},
\]

where

\[
c_5 = \left( c_4 2^{\frac{d}{\nu}} c_7 \left( 1 + \frac{d}{\nu} \right) + c_4 2^{\frac{d}{\nu}} c_7 \left( 1 - \frac{d}{\nu} \right) \right).
\]

If \( \alpha d > 2 \beta \nu \), we set \( n_l = \left[ \left( 2\epsilon^{-1} c_6 \xi_0 \frac{\alpha d - 2 \beta \nu}{2(\nu + d)} \right) (1 - T^{-\frac{\alpha d - 2 \beta \nu}{2(\nu + d)})^{-1} \right] \left( \frac{\xi_l}{\xi_0} \right)^{(\alpha + 2 \beta \nu) \frac{d}{2(\nu + d)}} \right] \) so that

\[
|f_\infty(x) - \hat{f}_L(x)| \leq \epsilon \frac{c_5}{2} \left( 1 - T^{-\frac{\alpha d - 2 \beta \nu}{2(\nu + d)}} \right) \sum_{l=1}^{L} \xi_l^{-\beta} \left( 1 - T^{-\frac{\alpha d - 2 \beta \nu}{2(\nu + d)}} \right) \left( 1 - T^{-\frac{\alpha d - 2 \beta \nu}{2(\nu + d)}} \right)^{-1} = \epsilon.
\]

3
To bound the computational cost $C_{\text{tot}}$, since the upper bound for $n_l$ is given by
\[ n_l \leq \left(2\epsilon^{-1}c_6\xi_0^{(\alpha-2\beta\nu)/(2(\nu+d))} (1 - T^{-\alpha-2\beta\nu/2(\nu+d)})^{-1}\right)^{2\beta} \xi_l^{(\alpha+2\beta\nu)/2(\nu+d)} + 1, \]
the computational cost is bounded by
\[
(S3.10) \quad C_{\text{tot}} \leq c_4 \sum_{l=1}^L n_l \xi_l^{\beta} \leq c_4 \left( c_6 \epsilon^{-2} \sum_{l=1}^L \xi_l^{(\alpha+2\beta\nu)/(2(\nu+d))} + \sum_{l=1}^L \xi_l^{-\beta} \right),
\]
where $c_8 = (2c_6^{\alpha-2\beta\nu/2(\nu+d)} (1 - T^{-\alpha-2\beta\nu/2(\nu+d)})^{-1})^{\frac{2\beta}{d}}$. By the standard result for a geometric series, we have
\[
(S3.11) \quad \sum_{l=1}^L \xi_l^{(\alpha+2\beta\nu)/(2(\nu+d))} = \sum_{l=1}^L \xi_l^{\alpha-2\beta\nu/2(\nu+d)} = \xi_0^{\alpha-2\beta\nu/2(\nu+d)} \sum_{l=1}^L T^{-\alpha-2\beta\nu/2(\nu+d)} \leq \xi_0^{\alpha-2\beta\nu/2(\nu+d)} \left(1 - T^{-\alpha-2\beta\nu/2(\nu+d)} \right)^{-1}.
\]
Thus, combining (S3.10), (S3.11) and (S3.9), it follows that
\[ C_{\text{tot}} \leq c_5 \epsilon^{-\frac{d}{\nu}}, \]
where
\[ c_5 = c_4 c_6 \xi_0^{(\alpha-2\beta\nu)/(2(\nu+d))} \left(1 - T^{-\alpha-2\beta\nu/2(\nu+d)} \right)^{-1} + c_4 2^{\frac{2\beta}{d}} c_1 \frac{\beta}{2(\nu+d)} \left(1 - T^{-\alpha-2\beta\nu/2(\nu+d)} \right)^{-1}. \]
If $\alpha d < 2\beta \nu$, we set $n_l = \left[ \left(2\epsilon^{-1}c_6\xi_0^{(\alpha-2\beta\nu)/(2(\nu+d))} (1 - T^{-\alpha-2\beta\nu/2(\nu+d)})^{-1}\right)^{\frac{d}{2\beta}} \xi_l^{(\alpha+2\beta\nu)/(2(\nu+d))} \right]$. Because
\[
(S3.12) \quad \sum_{l=1}^L \xi_l^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}} = \xi_L^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}} \sum_{l=1}^L (T^{-\alpha-2\beta\nu/2(\nu+d)})^{L-L} < \xi_L^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}} \left(1 - T^{-\alpha-2\beta\nu/2(\nu+d)} \right)^{-1},
\]
it follows that
\[ |f_\infty(x) - \hat{f}_L(x)| \leq \frac{\epsilon}{2} + \frac{\epsilon}{2} \xi_L^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}} \left(1 - T^{-\alpha-2\beta\nu/2(\nu+d)} \right)^{L} \sum_{l=1}^L \xi_l^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}}
\[ = \frac{\epsilon}{2} + \frac{\epsilon}{2} \xi_L^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}} \left(1 - t^{-\alpha-2\beta\nu/2(\nu+d)} \right) \sum_{l=1}^L \xi_l^{\frac{2\beta\nu-\alpha d}{2(\nu+d)}}
\[ \leq \frac{\epsilon}{2} + \frac{\epsilon}{2} = \epsilon. \]
To bound the computational cost $C_{\text{tot}}$, since the upper bound for $n_l$ is given by
\[ n_l \leq \left(2\epsilon^{-1}c_6\xi_L^{\alpha-2\beta\nu/(2(\nu+d))} (1 - T^{-\alpha-2\beta\nu/2(\nu+d)})^{-1}\right)^{\frac{d}{\nu}} \xi_l^{(\alpha+2\beta\nu)/(2(\nu+d))} + 1, \]
the computational cost is bounded by

\[(S3.13) \quad C_{\text{tot}} \leq c_4 \sum_{l=1}^{L} n_l \xi_l^{-\beta} \leq c_4 \left( c_9 \epsilon^{-\frac{d}{\beta}} \sum_{l=1}^{L} (\frac{(a+\beta)d}{2\nu+d})^{\frac{a-2\beta d}{2(\nu+d)}} \xi_l^{(a+\beta)d-\beta} + \sum_{l=1}^{L} \xi_l^{-\beta} \right), \]

where \(c_9 = (2c_6 \xi_L^{\frac{ad-2\beta d}{2(\nu+d)}} (1 - T^{-\frac{2\beta \nu-ad}{2(\nu+d)}}))^{\frac{2}{2}}.\) Because (S3.2) gives

\[\xi_L^{-1} < T \left( \frac{\epsilon}{2c_1} \right)^{-1/\alpha} \leq T^{2^{1/\alpha} c_1^{1/\alpha} \epsilon^{-1/\alpha}},\]

combining with (S3.12), it follows that

\[(S3.14) \quad \sum_{l=1}^{L} \xi_l^{(a+\beta)d-\beta} = \sum_{l=1}^{L} \xi_l^{\alpha-2\beta d} \leq \xi_L^{\frac{2\beta \nu-ad}{2(\nu+d)}} \left( 1 - T^{-\frac{2\beta \nu-ad}{2(\nu+d)}} \right)^{-1} \leq c_{10} \epsilon^{-\frac{d}{\beta} - \frac{2\beta \nu-ad}{2(\nu+d)}},\]

where

\[c_{10} = T^{\frac{2\beta \nu-ad}{2(\nu+d)}} \frac{2\beta \nu-ad}{2(\nu+d)} \frac{2\beta \nu-ad}{2(\nu+d)} \left( 1 - T^{-\frac{2\beta \nu-ad}{2(\nu+d)}} \right)^{-1}.\]

Thus, combining (S3.13), (S3.14), and (S3.9), and by the fact \(\epsilon^{-\frac{d}{\beta}} \leq \epsilon^{-\frac{d}{\beta}} \frac{2\beta \nu-ad}{2(\nu+d)}\) for \(\epsilon < \epsilon^{-1},\) it follows that

\[C_{\text{tot}} \leq c_5 \epsilon^{-\frac{d}{\beta} - \frac{2\beta \nu-ad}{2(\nu+d)}},\]

where

\[c_5 = c_4 c_9 c_{10} + c_4 \frac{2^\beta}{c_1} \frac{T^\beta}{1 - T^{-\beta}}.\]

**S4. Proof of Corollary 4.2.** By Condition 1 of Theorem 4.1 and Condition 1, it follows that

\[(S4.1) \quad |f_\infty(x) - f_H(x)| \leq c_1 \xi_l^{\alpha} \leq \epsilon/2.\]

Similar to Theorem 3.1,

\[(S4.2) \quad |f_H(x) - \hat{f}_H(x)| \leq c_{\Phi_H} \|\Theta_H\|^{\nu}_H \|f_H\|_{N_{\Phi_H}(\Omega)}\]

with a positive constant \(c_{\Phi_H}.\) Given Condition 2, similar to (S3.4), it can be shown that \(\|f_H\|_{N_{\Phi_H}(\Omega)} \leq c_{11} \xi_l^{\alpha/2}\) with a positive constant \(c_{11}.\) Combining with (S4.1), (S4.2), by Condition 4 of Theorem 4.1 and Condition 3, it follows

\[|f_\infty(x) - \hat{f}_H(x)| \leq |f_\infty(x) - f_H(x)| + |f_H(x) - \hat{f}_H(x)| \leq \frac{\epsilon}{2} + c_{12} n_H^{-\frac{\alpha}{2}} \xi_l^{\alpha/2}\]

with a positive constant \(c_{12}.\) Let \(n_H = \left\lceil (2\epsilon^{-1} c_{12} \xi_l^{\alpha/2})^{\frac{1}{2}} \right\rceil,\) then it can be shown that \(c_{12} n_H^{-\frac{\alpha}{2}} \xi_l^{\alpha/2} \leq \epsilon/2\) which leads to \(|f_\infty(x) - \hat{f}_H(x)| \leq \epsilon.\)
The bound the computational cost $C_{\text{tot}}$, since the upper bound for $n_H$ is given by

\[ n_H \leq \left(2\epsilon^{-1}c_{12}\xi^{\alpha/2}\right)^{\frac{d}{\nu}} + 1, \]

the computational cost is bounded by

(S4.3) \[ C_{\text{tot}} \leq c_4n_H\xi_H^{-\beta} \leq c_{13}\epsilon^{-\frac{d}{\nu}}\xi_H^{\frac{\alpha}{\nu}\beta - \beta} + \xi_H^{-\beta}, \]

where $c_{13} = (2c_{12})^{\frac{d}{\nu}}$. By Condition 1, it follows that

\[ \xi_H^{\frac{\alpha}{\nu}\beta - \beta} \leq \left(\frac{\epsilon}{2c_1}\right)^{\frac{d}{\nu} - \frac{\beta}{\nu}}, \]

and

\[ \xi_H^{-\beta} \leq c_1^{-\frac{\beta}{\nu}}\left(\frac{\epsilon}{2}\right)^{-\frac{\beta}{\nu} - \frac{d}{2\nu}}, \]

and combining the two inequalities with (S4.3), we have

\[ C_{\text{tot}} \leq c_{13}\epsilon^{-\frac{d}{\nu}}\xi_H^{\frac{\alpha}{\nu}\beta - \beta} + \xi_H^{-\beta} \leq c_{14}\epsilon^{-\frac{d}{\nu} + \frac{d}{2\nu} - \frac{\beta}{\nu}} + c_{15}\epsilon^{-\frac{d}{\nu} - \frac{d}{2\nu}} \leq c_{16}\epsilon^{-\frac{\beta}{\nu}} - \frac{d}{2\nu}, \]

where $c_{16} = c_{14} + c_{15}$, $c_{14} = c_{13}(2c_1)^{\frac{\beta}{\nu}\alpha - \frac{d}{2\nu}}$, and $c_{15} = c_{13}c_1^{\frac{\beta}{\nu}\alpha}2^{\frac{d}{2\nu} - \frac{\beta}{\nu}}$. This finishes the proof.