**Methodology of Simulated Enhanced Bayesian Optimization**

**1. Problem Setup**

This paper describes the implementation of the Simulated-Enhanced Bayesian Optimization (SEBO) framework, which is designed to solve systems design problems that utilize two types of experimental evaluations: (1) expensive but unbiased physical experiments, and (2) inexpensive, but biased computer simulations. SEBO aims to improve optimization efficiency by using physical data to calibrate a simulation model, then using the calibrated model to guide the selection of future physical experiments.

Let define a design space and a true system response function f(x) for any design . Observations from physical experiments are denoted as:

where is random observational error. The simulation model is an approximation of f(x) that includes both model bias and random error represented as:

where is a deterministic bias that is dependent on simulation parameters , and is stochastic error. The process is initialized with a set of n0 physical experiments that produce data points {(xi, yi)}.

**2. Simulation Model Calibration**

To align the simulation model with the results from performing physical experiments, parameters values **p** are calibrated by minimizing the squared difference between observed and simulated values. The following is solved:

using Bayesian Optimization (BO). Each iteration involves evaluating the loss function at a new parameter setting p, thus for each trial parameter vector p proposed by BO, a corresponding simulation experiment is run per physical data point already collected, making calibration increasingly expensive as more physical points are accumulated.

**3. Neural Network Surrogate Model Calibration**

After calibration, simulated data is generated by sampling N new points from the design space using Latin Hypercube Sampling (LHS) and evaluating each new point at . These points are used to train the Neural Network surrogate model. To quantify prediction uncertainty, Monte Carlo (MC) Dropout is used during inference, which yields predictive mean and standard deviation for any input design x.

**4. Metropolis-Hastings Sampling for New Physical Points**

For selection of promising candidate points for future physical experiments, an acquisition function is defined as:

The upper confidence bound (UCB) function balances exploitation (high predicted mean) and exploration (high uncertainty) of the neural network response. Metropolis-Hastings (MH) sampling is applied using q(x) as the target density to generate a set of new candidate points for physical evaluation. The MH sampler begins with the design points with the highest value.

The selected points from MH sampling are then evaluated through physical experiments and then appended to the original dataset. The process then iterates over again by recalibrating the simulation model with the updated dataset and proceeding with the previous steps.