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Bayesian Optimization for Automatic Reactor Design Optimization

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ABSTRACT:

Physics simulators have been widely used for performance prediction for nuclear reactor designs. However, running a simulation experiment is often very time-consuming, so it is critical to reduce the number of iterations in the design optimization procedure, to minimize the design cycle time.

This project aims to achieve this goal by implementing and configuring Bayesian Optimization (BO) method, a state-of-the-art approach in data science for zeroth-order sequential optimization on complex, high-dimensional response surfaces. Specifically, we use a Gaussian processes (GP) model to iteratively update the prediction and uncertainty evaluation for the relationship between the design variables (e.g., component shapes, material properties, etc.) and a performance metric based on the multi-physics simulation outputs. Based on past simulation runs, the BO method automatically suggests new design variables to acquire the responses, based on the existing response surface prediction and uncertainty evaluation, to quickly find the decision variables that achieve the optimal response value.

To accomplish this goal, we will first build multiple test cases for BO based on the models in the Virtual Test Bed, such as a heat-pipe micro-reactor. We will complete a tool chain that (1) automatically generates component shapes and mesh based on input design parameters, (2) perform the simulation experiment, and (3) evaluate the system performance index. Based on this tool chain, we will develop and evaluate BO capabilities for identifying the near-optimal reactor designs with a reduced number of simulation experiment runs. Finally, we will adapt the conventional GP models to address the key characteristics of nuclear reactor simulation. For example, we will explore automatic mesh-size determination by incorporating computing time into the acquisition function. We will enable the screening of insignificant groups of design inputs when the total number of design inputs is large, and explore using deep GP as the surrogate model to address the high-dimensional input design parameters. We will finally explore the modularized surrogate model of multi-physics coupling simulations, where each physics equation is described with a GP surrogate model, to fully utilize the physics information and all simulation output, thereby increasing the model accuracy and further decreasing the design cycle time.

In this collaborative project, the deliverables will be the test cases used for evaluating BO and other search-based design optimization approaches, validated BO methodologies for the reactor design application, new BO methodologies based on the system characteristics, and software modules for achieving efficient and automatic design selection and optimization. The PIs of this project will collaborate closely with the ongoing development of the stochastic tool's module of MOOSE.