Karlsruher Institut für Technologie

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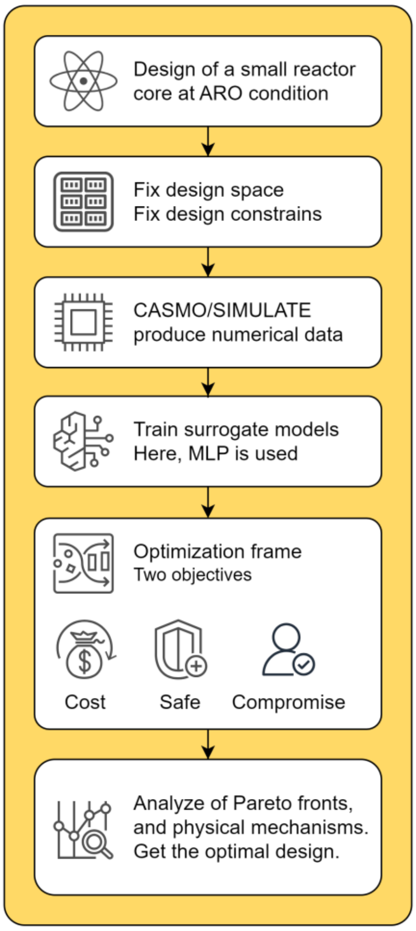
Master Work Proposal

Topic: Enhancement and Evaluation of an Active-Learning-Based Dual-Stage Multi-Objective Optimization Platform for Nuclear Core Design

Motivation

Small reactors are increasingly regarded as a viable solution for reliable and low-carbon energy generation. Their design, however, involves complex multi-objective optimization problems with high computational cost due to the reliance on numerical simulation tools. To address this challenge, advanced optimization frameworks integrating machine learning and evolutionary algorithms have been developed to improve efficiency and scalability.



An active-learning-based dual-stage Multi-Objective Optimization (MOO) system has already been established at KIT and successfully demonstrated on Small Modular Reactor (SMR) design problems. While the current platform shows strong performance, it relies on a specific set of methodological components (e.g., MLP and NSGA-II), whose optimality and generality remain open questions. Therefore, an enhancement and evaluation of the platform is necessary to further improve its robustness, accuracy, and adaptability.

Research Content

This project aims to enhance and evaluate the existing active-learning-based dual-stage MOO platform, with a focus on improving its machine learning models, optimization strategies, and uncertainty quantification capabilities. Unlike application-oriented studies, this work focuses on the methodology and performance of the optimization framework itself.

The current framework employs MLP surrogate models (regressor and classifier), the NSGA-II algorithm, and Sobol sampling methods. In this project, alternative and extended components will be investigated and integrated into the platform.

On the machine learning side, Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) will be explored to better capture spatial and structural correlations in reactor core configurations. These models may provide improved predictive performance compared to MLPs.

On the optimization side, NSGA-III and Multi-Objective Evolutionary Algorithm based on Decomposition (MOEA/D), may be implemented and compared with the baseline NSGA-II in terms of convergence behavior, diversity of Pareto fronts, and computational efficiency.

Furthermore, approaches such as Monte Carlo dropout will be investigated to approximate Bayesian inference in neural networks, enabling uncertainty estimation in surrogate predictions, together with the implemented ensemble method.

The performance of different configurations of the platform will be evaluated using representative reactor core design problems. Key aspects include optimization accuracy, computational cost reduction, robustness against surrogate errors, and efficiency of the active learning process.

Work Plan (6 months, flexible)

1) Study the existing optimization platform, including its architecture, workflow, and validated SMR application case.
2) Implement and integrate alternative surrogate models (e.g., CNN, GNN) into the framework.
3) Implement alternative multi-objective optimization algorithms (e.g., NSGA-III, MOEA/D).
4) Extend the framework with uncertainty quantification techniques (e.g., Monte Carlo dropout) and adapt the active learning strategy accordingly.
5) Analyze results and identify key factors influencing performance, leading to recommendations for future development of the optimization system.

Skill Requirements

- Nuclear engineering background with knowledge of reactor physics and safety considerations.
- Understanding of machine learning principles and basic optimization methods.
- Programming skills in Python for workflow automation, optimization, and data analysis.
- Ability to understand and extend complex computational workflows.

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