Concurrent Surrogate Model Development with Uncertainty Quantification in the MOOSE Framework Using Physics-Informed Gaussian-Process Machine Learning

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ABSTRACT:

Multiscale and multiphysics modeling and simulation (M&S) provide a means of combining high-fidelity simulations that capture lower length-scale (LLS) behavior with higher length-scale (HLS) simulations. These approaches are regularly used for nuclear reactor simulation and the open-source MOOSE framework has emerged as a popular means of enabling multiscale and multiphysics reactor simulations. Traditionally, multiscale M&S is carried out in one of two ways: concurrent coupling or hierarchical coupling, illustrated in Fig1(a). Concurrent coupling pays the computational cost of the LLS simulations every time the HLS simulation is run, while hierarchical coupling pays the cost before the HLS simulations. However, the range of conditions experienced during the HLS simulation is not known ahead of time, which can result in either an insufficient number of LLS simulations increasing error, or too many LLS simulations wasting computational cost.

The objective of this project is to develop a general capability for concurrent generation and use of physics-informed Gaussian process (GP)-based surrogate models to facilitate multiscale and multiphysics modeling. HLS simulations will use the surrogate models and when their uncertainty estimates are too high, LLS simulations will be launched, and the surrogate models will be improved. We will implement this new capability as part of the Multiphysics Object-Oriented Simulation Environment (MOOSE) so that every application based on the MOOSE framework will have access to it. We will evaluate and enhance the GP-based surrogate models using three reactor-relevant test cases that each represent a common type of multiscale problem:

- Fission gas diffusivity in doped UO_2,
- Creep in metallic cladding,
- TRISO particle behavior in particle compacts.

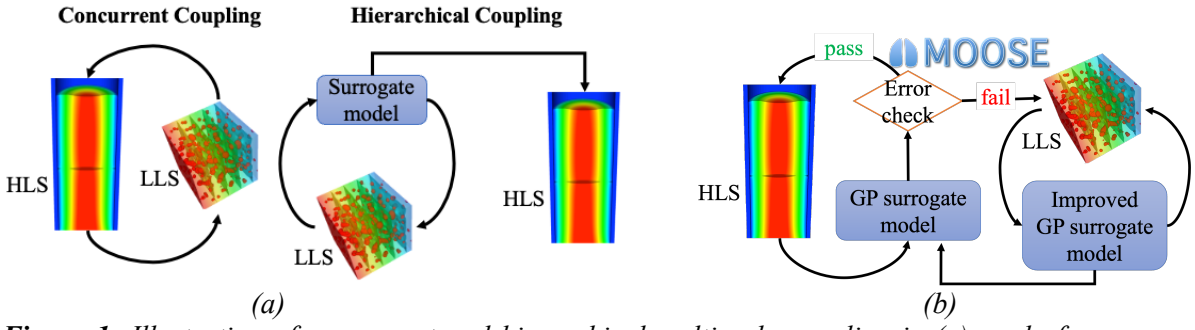

***Figure 1**: Illustration of concurrent and hierarchical multiscale coupling in (a), and of our proposed multiscale concurrent GP surrogate model capability for MOOSE in (b)*