



Abstract

Title: Physics Model Calibration via Functional Kernel Regression.

Authors:

1. *Kwesi Appau Ohene-Obeng - Department of Mathematical Science, University of Texas at El Paso, El Paso, Texas*
2. *Xiaogang Su, Ph.D. - Department of Mathematical Science, University of Texas at El Paso, El Paso, Texas*
3. *Salil Koner, Ph.D. – Statistics Department, University of California, Riverside*

We propose a comprehensive methodology for physics-based model calibration that integrates functional data analysis with neural network surrogate modeling to address the statistical and computational complexities inherent in large-scale high-fidelity simulation experiments. Leveraging both field experimental observations and large-scale simulation outputs, the proposed framework models spatially and temporally indexed functional responses arising from complex physical systems, including aerodynamic flow dynamics and radiative shock hydrodynamics. A flexible modeling structure is developed within the functional data analysis paradigm to capture underlying functional variation, accommodate heterogeneous measurement patterns across non-uniform observational grids, and represent both smooth and locally complex behavior in the observed responses across irregular spatial and temporal domains.

For input parameter calibration, we introduce a functional kernel regression approach that maps discrete noisy observations into continuous functional representations via penalized B-spline basis expansions with data-driven smoothing parameter selection through generalized cross validation. This representation enables the construction of a coefficient-based L^2 distance metric in the space of B-spline coefficients, which rigorously reduces the infinite-dimensional functional calibration problem to a tractable finite-dimensional estimation setting. A deep feedforward neural network surrogate with Monte Carlo Dropout regularization is trained to emulate the functional simulator output across the joint design and calibration parameter space, enabling principled uncertainty propagation through the calibration pipeline via repeated stochastic forward passes. Kernel regression is subsequently applied within this reduced coefficient space to estimate unknown calibration parameters by exploiting functional similarity between simulated and experimentally observed responses, yielding a computationally efficient and statistically principled estimator. The proposed framework is evaluated against established competing methodologies and demonstrates competitive parameter recovery with substantially reduced computational overhead, yielding stable and accurate parameter estimates across multiple experimental configurations and physical modeling environments.

Keywords: *Physics-Based Model Calibration, Functional Data Analysis, Penalized B-Spline Smoothing, Functional Kernel Regression, Neural Network Surrogate*