

Predicting Discontinuous and Long-Tailed Physical Fields via Tail-Aware Mixture of Experts

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ABSTRACT

In engineering design, accurate surrogate modeling of 3D physical fields is crucial for rapid design optimization. However, complex industrial parts often exhibit discontinuous physical behaviors (e.g., weld lines) and long-tailed data distributions, where critical defects are rare but fatal. Conventional regression models, including Deep Operator Networks, often suffer from "smoothness bias," failing to capture these sharp transitions and underestimating extreme values in the tail of the distribution.

To address these challenges, we propose a novel Regime-aware Mixture of Experts (MoE) framework combined with Tail-Aware Optimization. Our approach consists of three key components: (1) Regime Identification using unsupervised Gaussian Mixture Models (GMM) to soft-cluster physical behaviors into distinct regimes; (2) A Field Router Network, which dynamically assigns expert sub-networks to specific regimes based on local geometry and Fourier features; and (3) Tail-Aware Optimization, integrating Class-Balanced Weighting and Distribution Matching Focal Loss to amplify the learning signal for rare, critical events.

We validate our method on 3D Molded Case Circuit Breakers (MCCB), injection molding and structural analysis datasets. As shown in Fig. 1, the results demonstrate that our model significantly outperforms global regression baselines in capturing sharp boundaries of weld lines and predicting extreme values of sink marks. Future work will focus on integrating graph-based topological reasoning to handle variable mesh topologies and extending the framework to multi-fidelity learning.

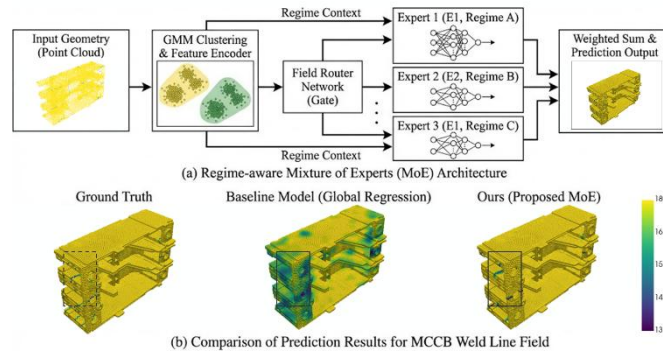


Figure 1: (a) The proposed Regime-aware Mixture of Experts (MoE) architecture with dynamic routing based on GMM clustering. (b) Prediction comparison for the MCCB weld line field. Our method (right) accurately captures discontinuous boundaries and tail extremes, whereas the baseline (middle) suffers from smoothness bias.

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