Machine Learning Surrogates for Phase-Field Modeling of Dendritic Metal Solidification

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The dendritic solidification of metals plays a critical role in determining the final microstructure and, consequently, the mechanical properties of components produced through additive manufacturing [1]. The phase-field model is a widely adopted computational framework for simulating microstructural evolution, capable of capturing complex interfacial dynamics such as dendritic growth, phase transformations, and pattern formation in alloys [2], [3]. Accurate prediction of microstructural evolution is essential for controlling and optimizing material performance, yet traditional phase-field simulations are computationally expensive, particularly when exploring wide design spaces or varying processing conditions. In this context, machine learning-based surrogate models have emerged as promising tools to approximate the spatio-temporal dynamics of dendritic solidification [4], enabling rapid and efficient evaluations without compromising physical fidelity. This work investigates various surrogate modeling strategies, including classical approaches based on XGBoost and convolutional neural networks, as well as hybrid classical-quantum models using variational quantum algorithms, assessing their ability to reduce computational cost, maintain microstructural prediction accuracy, and ultimately inform decision-making in advanced additive manufacturing processes. To make surrogate modeling a practical alternative to high-fidelity simulations, several challenges must be addressed. In particular, the spatio-temporal nature of dendritic growth requires models capable of capturing both spatial morphology and temporal evolution while minimizing dependence on costly simulation outputs. Moreover, the efficiency of surrogate models strongly depends on how training data are generated and selected, as shown in Figure 1. In this work, we investigate uncertainty-driven adaptive sampling strategies to reduce the number of required phase-field simulations, examine how the selection of temporal training instances affects predictive performance and potential computational savings [5]. Additionally, we explore hybrid classical–quantum regression based on Variational Quantum Algorithms as an emerging alternative for surrogate modeling in computationally expensive physical problems. Together, these efforts aim to enable accurate, data-efficient, and scalable prediction of dendritic microstructure evolution in metal solidification processes. To efficiently approximate dendritic solidification while minimizing reliance on costly phase-field simulations, two sampling strategies and four surrogate modeling approaches were evaluated. For sampling, a classical strategy based on Optimal Latin Hypercube Sampling (OLHS) optimized via Particle Swarm Optimization ensured uniform exploration of the design space, while an uncertainty-guided adaptive sampling strategy targeted regions of high model uncertainty (see Figure 2) to reduce the number of required training samples. Four surrogate models were considered: (i) a standard convolutional neural network (CNN), (ii) a domain-informed feature extraction approach combined with XGBoost (XGB), (iii) a self-supervised CNN leveraging a variational autoencoder for feature learning, and (iv) a hybrid classical–quantum model (VQA) using the same domain-informed features. In addition, the impact of temporal instance selection on model performance and computational efficiency was analyzed, balancing the number of phase-field snapshots required for inference with surrogate accuracy. In particular, when the final temporal instance used for inference is t_f, the phase-field model must be simulated up to t_f before the surrogate can be applied, which reduces potential computational savings; therefore, the minimal set of temporal instances necessary to maintain high predictive performance while minimizing dependence on the original phase-field simulations was also investigated. The evaluation of surrogate modeling strategies for dendritic solidification has demonstrated that classical machine learning approaches can achieve accurate prediction of microstructural evolution while substantially reducing the computational cost associated with high-fidelity phase-field simulations. Adaptive sampling strategies were shown to improve sample efficiency compared to classical uniform sampling, particularly for convolutional models, which are capable of learning spatial representations directly from data and achieve competitive performance with a reduced number of samples. This property is especially valuable when extrapolating to more computationally demanding phase-field problems, such as high-resolution 2D or fully 3D simulations, where generating training data is significantly more expensive. Domain-informed feature extraction combined with XGBoost provided the best overall balance between accuracy and training cost, whereas CNNs, especially when combined with adaptive sampling, offered greater generalization in scenarios with limited prior knowledge. Analysis of temporal instance selection revealed that including snapshots closer to the target solidification state improves predictive accuracy but incurs higher computational cost, highlighting a trade-off between model performance and reliance on phase-field simulations. Hybrid classical–quantum approaches, such as Variational Quantum Algorithms (VQAs), were also explored, demonstrating the potential of emerging quantum methodologies to address surrogate modeling challenges. However, their performance remains limited due to convergence difficulties arising from highly non-convex and high-dimensional parameter spaces, as well as constraints on the number of test cases that can be explored both in simulators and on current NISQ hardware. While VQAs show promise as an area of ongoing research and may improve with further advances in circuit design and optimization strategies, they are not yet competitive with classical methods in terms of accuracy, scalability, or robustness. Overall, these findings confirm that surrogate modeling provides a practical and scalable route to efficiently predict microstructural evolution, inform process optimization, and reduce computational and environmental costs, while continued developments in both classical and quantum methodologies are expected to expand applicability in industrial contexts.

References

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Figures

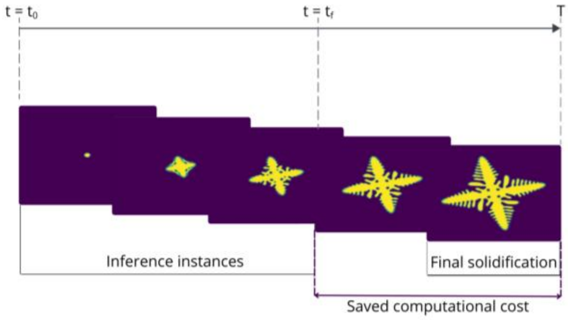

Figure 1. Computational dependence between the selected inference instances and the original phase-field model.

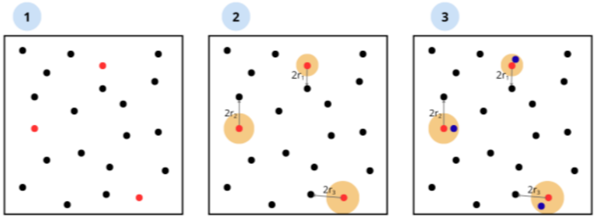

Figure 2. Uncertainty guided adaptive sampling. Red dots indicate most uncertain samples, and blue dots indicate the new samples. Hyperspheres are defined under the assumption of locally preserved uncertainty around each point.