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OPTIMIZING NEURAL NETWORK MODEL FOR ACCURATE PREDICTION OF THERMAL HISTORY DURING LASER DIRECT ENERGY DEPOSITION OF Ti-6Al-4V

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ABSTRACT

As deep neural networks (DNN) become more prominent, they require large amounts of data, making it challenging for the laser direct energy deposition (LDED) process of Ti-6Al-4V applications. However, integrating the physical knowledge into the DNN architecture represents a significant advancement in predictive modeling for the LDED process of Ti-6Al-4V. This approach addresses the complex interplay of thermal dynamics and material properties, crucial for product quality and integrity. Therefore, Physics-constrained NN (PCNN) is proposed by integrating physical knowledge as regularization terms within the overall loss functions of the DNN model. The multi-fidelity method used for training, which combines low-fidelity and high-fidelity networks, improves training efficiency by narrowing the search space and directing the training process more effectively. Training efficiency by multiphysics models is enhanced through two main strategies: employing a more efficient thermo-mechanical data-gathering approach (finite element method-FEM) and leveraging the thermo-fluid model (phase field-thermal lattice Boltzmann method) to facilitate the efficient use of physical constraints for better guidance. The proposed PCNN showcases its applicability by predicting thermal history. The PCNN models demonstrate superior accuracy over the traditional DNN. The comparison between PCNN predictions and FEM simulations reveals a significant relationship in predicting the thermal history between critical points within printed parts, such as the substrate and successive layers. Despite minor variances, particularly at peaks, the PCNN predictions closely align with FEM observations, indicating the model's capability to replicate complex thermal behavior. These findings underscore the importance of integrating physical knowledge into DNN, to enhance predictive performance and efficiency in complex simulations for LDED process applications.

KEYWORDS

Deep neural network, finite element method, phase field – thermal lattice Boltzmann method, laser direct energy deposition, Ti-6Al-4V, thermal history.

INTRODUCTION

The LDED process has emerged as a promising manufacturing process for producing complex alloy parts, like Ti-6Al-4V (Ansari et al., 2021). The LDED process offers significant advantages in terms of design flexibility and material efficiency (Paul et al., 2021). However, thermal distributions and cooling rates experienced by the Ti-6Al-4V during printing play a crucial role in determining the final microstructure and mechanical properties of the printed parts (Moeinfar et al., 2022). As a result, accurate prediction of the thermal history is essential for ensuring consistent, high-quality outputs.

Multiphysics models enhanced the accuracy of simulations by addressing the complex interplay of various physical processes involved (Bayat et al., 2021). However, multiphysics models face significant limitations. Thermo-mechanical finite element model (FEM) while capable of providing detailed results, simulates thermal strain, residual stresses, and distortion (Singh et al., 2022), does not capture micro-scale making it impractical for real-time process control. Furthermore, the thermo-fluid phase field-thermal lattice Boltzmann models (PF-TLBM) integrate thermal analysis with fluid flow dynamics to simulate melt pool behavior, heat transfer, and solidification (Rahman, 2020; Rahman et al., 2021), but do not capture the macro scale. This creates a need for a predictive method that can balance accuracy and computational efficiency while accounting for the intricacies of the LDED process for Ti-6Al-4V.

NN models have shown promise in various manufacturing applications due to their ability to handle complex geometries and their potential for rapid computation once trained (Abiodun et al., 2019). However, the NN potential for accurately predicting thermal history in the LDED of Ti-6Al-4V has not been fully optimized. This limitation stems primarily from the significant challenges in collecting large, high-quality datasets required for effective training, given the intricate and costly nature of the LDED process. To overcome these challenges for predicting thermal history in LDED of Ti-6Al-4V, innovative approaches are necessary. Therefore, the primary objective of this paper is to optimize the NN model that can accurately predict thermal history while effectively addressing data limitations.

MATERIAL AND METHODOLOGY

Integrating physical knowledge into the DNN model during data regularization is proposed to predict the spatiotemporal evolution of the thermal field of Ti-6Al-4V during the LDED process. The stages of the proposed PCNN model are illustrated in Figure 1. The first stage is data collection through the FEM and PF-TLBM, followed by the developing DNN architecture, the next stage is training and evaluation of the proposed PCNN model, and lastly predictions.

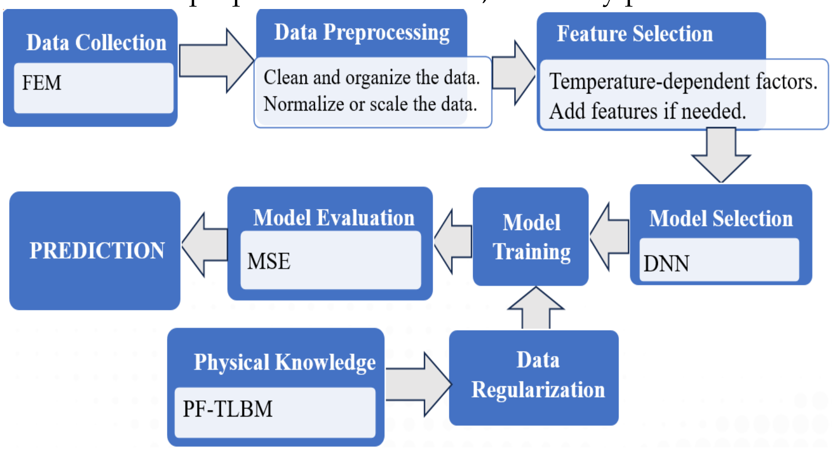

Figure 1: The stages involved in the proposed physics-constrained neural network.

RESULT AND DISCUSSION

Table 1 shows a comparison of deep neural networks and physics-constrained neural networks for the thermal field. Notably, by one order of magnitude, the MSEs for PCNN are significantly lower than DNN. The PCNN exhibits a balanced loss across the board. It also emerges as the top performer in terms of prediction accuracy while also taking the highest amount of training time. However, it is essential to remember that the training of the PCNN requires a greater amount of computational time than the DNN. This is because the PCNN incorporates physical knowledge. Additionally, the data showed that the PCNN model outperforms the DNN, with an accuracy rate close to 98.09%. DNN has the lowest accuracy at 75.40\%, which suggests it might be less suitable for the prediction of the evolution of thermal field during LDED of Ti-6Al-4V.

Table 1: Comparison of deep neural network and physics-constrained neural network for the thermal field.

NN Models	Training Time (s)	MSE of Prediction at t = 0	MSE of Prediction at t = 1	Accuracy (%)
DNN	8.66	0.0293	0.1998	75.40
PCNN	1019.07	0.0055	0.0139	98.09

Figure 2 illustrates the comparison of convergence rates between the DNN and the proposed PCNN based on the volume of training data. The superiority of PCNN over DNN is more pronounced under conditions of scarce training data, with prediction accuracy differences reaching up to an order of magnitude for training datasets smaller than 400. To attain a precision level of 0.01, DNN necessitates around 900 training samples, whereas PCNN requires merely about 300, demonstrating the PCNN's higher efficiency and the significant benefit of incorporating physical knowledge into the model.

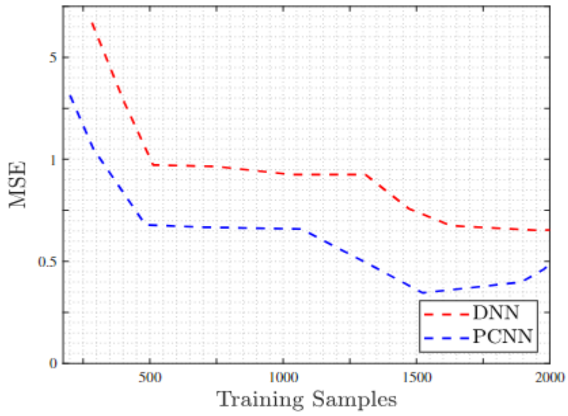

Figure 2: Convergence analysis between DNN and PCNN.

Figure 3 illustrates the comparison between FEM and predicted PCNN for the entire deposition. From 0-125s, both models show a constant low temp. around 500K, indicating a preheating before the active deposition begins. Starting at 125s, there are sudden, intense temp. rise reaching up to 1800K, followed by sharp drops. These spikes show laser heating during the deposition of individual layers. The maximum temperature of each spike gradually decreases over time, from 1800K to 1200K, suggesting heat accumulation in the part as the build progresses. The minimum temp. between peaks slowly increases from 500K to 800K, indicating overall heating of the workpiece throughout the deposition process.

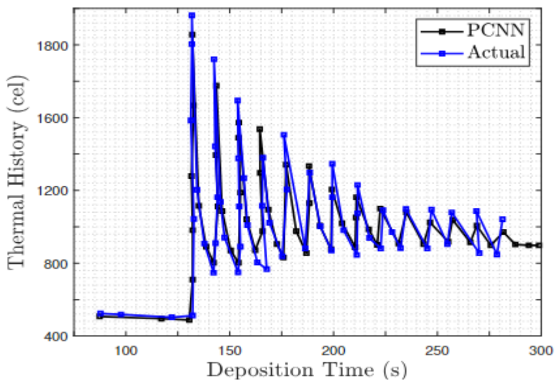

Figure 3: Comparison between FEM and predicted PCNN for the entire deposition.

CONCLUSION

Integrating physical knowledge into DNN models marks a significant advancement in predictive modeling for the LDED process of Ti-6AI-4V. This approach addresses the complex interplay of thermal dynamics, which critically affect the quality and integrity of the final product. By integrating the fundamental insights from the multiphysics model into the adaptability and pattern recognition capabilities of DNNs, a robust predictive framework was created. This integration enhances predictive accuracy and provides deeper insights into the intricate interactions within the LDED process of Ti-6AI-4V. The inclusion of physical principles ensures that predictions are grounded in physics, capturing nuanced behaviors of thermal fields. This combined approach not only improves predictive accuracy but also informs decision-making to minimize defects, optimize material properties, and enhance manufacturing efficiency.

The quantitative comparison and analysis of DNN highlight the superior performance of the PCNN models in terms of training duration and prediction accuracy. The PCNN models require more computational time due to the integration of physical knowledge, and the higher accuracy rates near 98.09%, demonstrate their suitability for predicting the thermal history during the LDED process of Ti-6Al-4V. The model loss analysis further supports this, with the PCNN showing rapid initial learning, better capacity for learning from the training dataset, and more effective generalization to new data compared to the DNN. The comparison between PCNN predictions and FEM simulations reveals a significant relationship in predicting the thermal history between critical points within printed parts, such as the substrate and successive layers. Despite minor variances, particularly at peaks, the PCNN predictions closely align with FEM observations, indicating the model's capability to replicate complex thermal behavior.

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