Multi-layer Thermal Simulation of Directed Energy Deposition using Physics Informed Neural Networks

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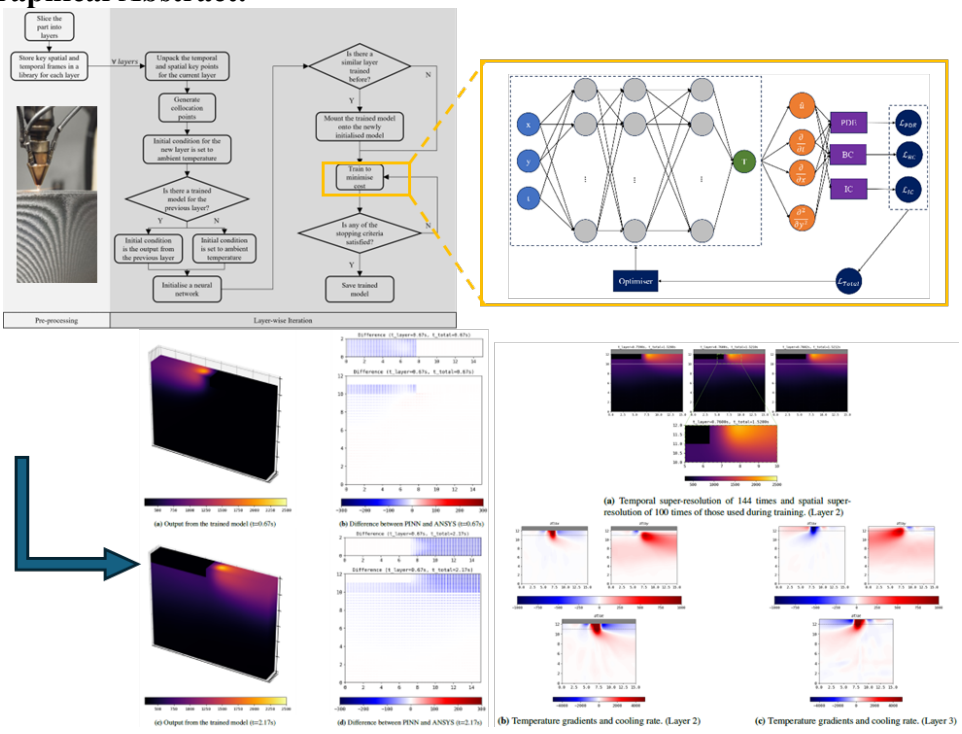
Abstract
This paper presents a physics-informed neural network (PINN)-based solution framework that predicts the thermal history during a multi-layer Directed Energy Deposition (DED) process. The meshless nature and the readily available derivative information of PINN solution opens up new opportunities for modelling the thermally induced distortion in metal Additive Manufacturing (MAM). The proposed framework incorporates simple yet effective strategies that enable PINN to overcome the usual shortfall of neural networks (NNs) in dealing with discontinuities, critical for applying PINN to the multi-layer problem due to DED's layer-by-layer nature. The accuracy of the proposed framework is validated via a benchmark test against ANSYS simulation. Leveraging the possibility of initialisation with prior knowledge, PINN is also demonstrating potential computational time-savings, especially for larger parts. The proposed framework sets the foundation for the subsequent exploration of applying scientific machine learning (SciML) techniques to real-life engineering applications.

Graphical Abstract:



1. Introduction

During the common MAM processes, the feedstock or the layer of powder is melted with a local heat source and re-solidifies to form the designed part geometry. Such a process involves steep thermal gradients and high cooling rates, resulting in multi-scale impacts on the final product – from impacts on mechanical properties to part distortion [1]. Hence, there is no shortage of attempts to predict the thermally induced phenomena in the literature, mainly numerically, and the common trade-off between fidelity and computational time is present [2]. By homogenising the scan patterns over multiple layers, quick computation can be achieved with a reasonable level of accuracy after proper calibration for the material and process, exemplified by the series of work on the modified inherent strain method [3], [4].

The rapid progress in machine learning (ML) algorithms and the enabling hardware have led to a significant uptake of ML-based surrogate modelling in many traditionally computationally intensive areas, including the field of MAM [5]. The concept of SciML which aims to incorporate physical laws into the training process of the ML models is gaining popularity for its potential of overcoming the stigma of 'black-box' in purely data-driven ML methods, with PINN [6] being one of the most adopted approach. In the field of MAM, many attempts on applying PINN focus on the single-layer problem [7].

In this article, we present our recent work in applying PINN to a multi-layer framework that emulates the DED manufacturing process, allowing part-scale, meshless thermal history prediction [8]. The proposed framework incorporates strategies that make PINN contiguous with the discontinuities in simulating the multi-layer DED process without labelled data over the simulated duration. Computational gains supported by initialisation based on a previously trained model, especially for large parts, are also explored. The authors envision that the proposed framework lays the foundation for the progression from geometry-only to process-aware design optimisation for DED.

2. Methodology

PINN, a type of SciML-based method, is used as a forward solver for the temperature history during the DED process and the graphical abstract illustrates the architecture of the NN employed. At the core of PINN, the auto-differentiation capability of an NN is utilised to obtain the respective terms in the governing equations. It subsequently allows the 'physics-informed' loss terms to be computed and used in the training process.

The governing equations used to construct the physical losses are based on the conduction model and the total loss term is the weighted sum from the PDE, BC, and IC losses. Due to the limited pages, full definition of the governing equations (including those for the 3D case) can be found in [8].

Without data, the model trains to determine the solution of the heat transfer equation by sampling the physical losses at the collocation points. The sensitivity of the training outcome with regard to the distribution and density of collocation points has been well documented in the literature. In our implementation, an increased PDE collocation point density is adopted to capture the localised heating. Illustration and more details can be found in [8].

To account for the discontinuity in initial condition for the multi-layer cases as well as to overcome the challenge for convergence, the following strategies are incorporated. Full details on the implementation of the strategies can be found in in [8]:

1. Pointwise-weight assignment for IC: large IC loss values are contributed by the collocation points close to the interface between the new layer of room temperature and the printed part with residual temperature (i.e. the discontinuity). To prevent completely losing the information closer to the interface but also reduces the magnitude of the error values which smoothens the loss topology and allows the training to continue, pointwise weight is assigned to the points close to the interface by $w_{i,IC}^{*} = \frac{1}{e^{-\alpha_w(|y_i - y_{interface}| - \beta h_{layer})}}$ where h_{layer} is the layer thickness, α_w and β are parameters controlling how fast and where the pointwise weight starts to decay to 0, respectively.
2. Training with causality: Incorporating causality in the training is proposed in [9] where the authors show that standard training of PINN is 'implicitly biased towards first approximating PDE solutions at later times', necessitating a training strategy that focuses on satisfying the solution in the correct temporal sequence (i.e. causality). It is identified that causality has a critical role in the multilayer problem since the correct solution of each subsequent layer depends on correctly capturing the initial condition which itself is challenging. The full definition of the causality implementation can be found in [8].

3. Results and Discussion

Figure 1 illustrates the comparison between the PINN result and that from ANSYS M-APDL simulation. The under-prediction of the core temperature compared to ANSYS benchmark result reveals a key artefact of the NN-based solution – the extrema are less sharply defined due to training cost being defined as weighted mean values from all collocation points. Hence, the extrema are smoothened in the approximation. Nevertheless, the underprediction is limited to within 10% in magnitude and within close proximity of the melt pool.

The super-resolution capability stemming from the meshless nature and the immediate availability of derivative information are two unique characteristics of PINN solutions and they are illustrated in Figure 2. It implies two potential

benefits – 1) the training time could be further reduced by adopting a coarser discretisation for collocation point assignment; 2) investigation at a much finer spatial and/or temporal scale can be conducted which is critical for a highly transient problem such as during DED or other metal AM processes.

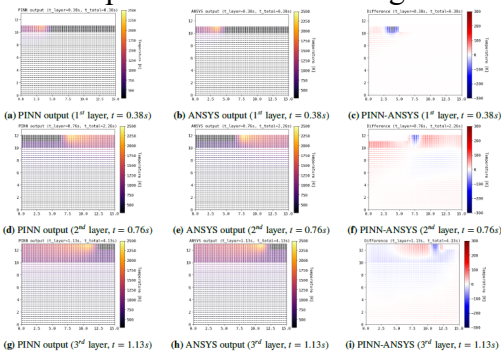


Figure 1: Benchmark comparison between the PINN and ANSYS simulations. A root mean square error of 20.48K, 41.31K, and 47.88K is observed for the 1st, 2nd, and 3rd layers, respectively.

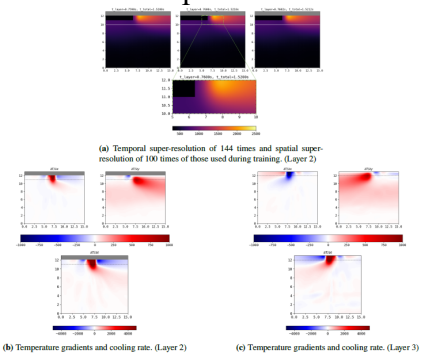


Figure 2: Demonstration of spatiotemporal super-resolution and availability of derivative information from the trained PINN model.

While the initial training for PINN may take longer than numerical simulations, time-saving could be achieved for larger parts with multiple layers where the training for the later stage is initialised based training model instead of from random. Figure 3 demonstrates the reduced total computing time for a 10-layer part.

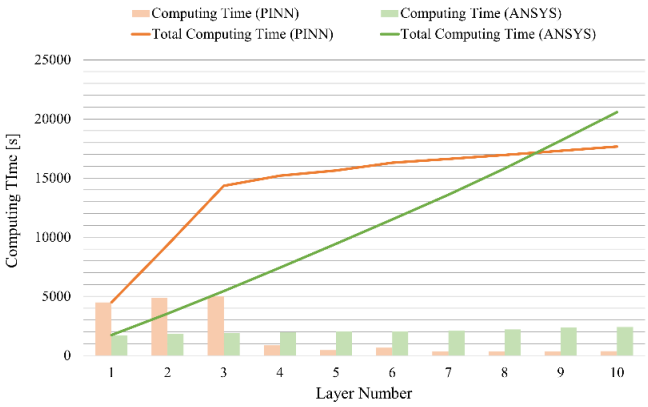


Figure 3: Computational time comparison between PINN and ANSYS.

Table 1: Density of collocation points and the associated RMSE in 2D and 3D cases

		2D			3D	
		Number of collocation points	**Planer/edge density**	**Equivalent volume/face density**	**Number of collocation points**	**Volume /face density**
PDE	**Global**	35	0.212	0.0977	330	1.00
	Secondary	165	2.20	3.26	330	2.20
	Local	704	29.3	159	1727	72.0
	sub-total	904	5.48	12.80	2387	7.23
BC	**sub-total**	67	1.34	1.80	400	1.00
IC	**sub-total**	2520	15.3	59.7	2640	8.00
RMSE [K]			20.48		19.42	

The framework can easily be extended to 3D. More importantly, while collocation points resemble mesh points, they do not necessarily scale with dimensions. Table 1 shows the comparison between the 2D and 3D collocation density. An illustration of the output from PINN and comparison against ANSYS result for a 3D case can be found in the graphical abstract.

4. Conclusion

Benefiting from strategies that make NN contiguous with the discontinuities that are intrinsic to the DED process, i.e. the pointwise weight assignment for IC loss and explicit definition of the solid-void regions, the proposed framework is able to achieve a similar level of accuracy as the numerical methods with the potential of significant time-saving for large-scale parts. Such a framework sets the foundation for employing PINN in the thermomechanical simulation for practical DED applications. Instead of acting as a replacement for conventional numerical methods, PINN's unique capability of incorporating both physical laws and experimental data implies that the proposed framework can either achieve continuous improvement in prediction when combined with data (e.g. from in-situ monitoring) as a forward solver, or be applied to the inverse problem where effective thermal properties are generalised from experimental observations, allowing computationally cheap, conduction-based numerical models to be utilised while maintaining good agreement with observations. Moreover, PINN models not only generate temperature history but also thermal gradients and cooling rates. Such information can be of use for alternative mechanical models that predict the thermally induced distortions on the fly. It opens up the possibility of optimisation with regard to thermal distortion which is an extremely exciting field of research

5. References

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