A Proposal for Physics-Informed Quantum Graph Neural Networks for Simulating Laser Cutting Processes

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Abstract: Simulations are crucial for production monitoring and planning in manufacturing. Still, the performance of simulations based on mathematical modeling and machine learning methods is limited and opaque to widespread application. Quantum computing offers the potential for exponential acceleration of these tools, while physically informed neural networks (PINN) improve learning and reduce ambiguity. Objective of this paper is to explore the concept of developing a tool for laser cutting simulation based on a quantum neural network that can be trained on thermal physics principles.

Keywords: Quantum Computing; PINN; Graph Neural Network; Predictive Simulation

1 Introduction

Laser cutting is a widely embraced manufacturing technique, e.g., in automotive. During the cutting process, thermal effects can lead to undesired outcomes such as distortion, and alterations in material properties; impacting the structural integrity and quality of end products. The process requires a balance of cutting speed, precision, and preserving edge quality. Analytical- or AI-based thermal simulations assist process optimization and design validation allowing manufacturers to make informed decisions. Still, these approaches often lack critical validation and present uncertainty due to oversimplification of the material's properties and boundary conditions [PH14]. The utilization of multiphysics modelling to simulate diverse conditional processes has a supportive effect but requires heavy computational power [Kn21]. Model-driven (i.e. ML) methods require less computational complexity but only reduce the maximum deformation by approx. 33% [Lu22]. Demonstrations showed that incorporating physics-based principles with neural networks (NN) enables them to capture the intricacies of the simulation, resulting in a faster-converging training process [RPK19]. These networks reduces dependence on input data by incorporating physical laws to help overcome learning plateaus. Thermodynamics-informed Graph NN (TIGNN) [He22] is one example of PINNs that successfully simulates fluid and metal changes exploiting Hamiltonian Physics. Using such methods can be a powerful tool for simulating the time-dependent and dynamic nature of the laser-cutting process. However, these solutions are often too resource-intensive whereas Quantum computing can offer great exponential speedup. Related work shows evidence of Quantum Machine Learning (QML) surpassing

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its classical counterparts [ZJQ23]. Given the criticality of speed and precision in laser cutting simulations, quantum-enhanced simulations hold the potential to ensure accurate component reproduction. This paper proposes a model to optimize the accuracy, efficiency, and effectiveness of laser cutting simulations by utilizing physics-based solutions and leveraging the capabilities of QC.

2 Proposed method

We aim to train a NN model to solve the partial differential equations governing the behaviour of a continuous laser beam source on a 2D rectangular plate. The temperature u(x,y,t) for this satisfies the following partial differential equation with initial and boundary conditions:

$$\frac{f-q}{\Delta z} = \rho c_p . \frac{\partial u}{\partial t} - \nabla(k.\nabla u)$$
$$q(x,y,t) = h.(u(x,y,t) - u_\infty)$$
$$u(x,y,0) = u_\infty, u(0,y,t) = u(a,y,t) = u(x,0,t) = u(x,b,t) = u_\infty$$

To enforce the model's learning process based on these rules, an additional losss function will be constructed that can be incorporated alongside the classical loss function. This model will be then transformed into a Quantum version of the PINN model. In typical QML approaches Parameterized Quantum Circuits [Be19] adopt the concept of setting predefined parameters and designing a gated parameterized model. The free parameters of the gates are adjusted using classical computing techniques which greatly simplifies the parameter-tuning process. The proposed structure to implement Physics-informed GNNs as Quantum based PINNs is inspired from a general implementation of quantum based PINNs [VB23].

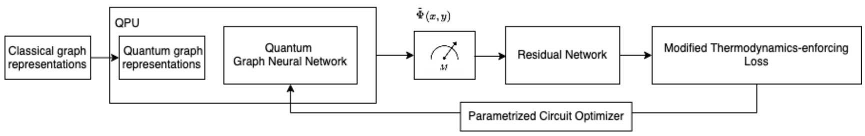

Abb. 1: Proposed circuit for Quantum-based PINN; illustration based on [VB23]

3 Conclusion

In this paper, we propose an idea to achieve improved performance in simulating the complex dynamics of laser-cutting processes, by harnessing the computational power and unique properties of QC. To implement the experiment, we will first encode the two-dimensional coordinates for the QNN unlike the one-dimensional cases introduced in previous works [Ma22]. After designing the tools to translate classical graph representations to quantum graph ones and vice-versa, the physics-based optimization will take place to generate the final model. The ultimate aim is to push the boundaries of QC further with PINNs to achieve trustworthy and effective simulation models for the manufacturing industry.

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