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Joint Optical–Thermal Optimization of Laser Processing Parameters Using Bayesian Optimization and Neural Emulators

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Abstract: *The precise control of laser material processing, particularly in regimes such as laser welding, cutting, and additive manufacturing, necessitates a rigorous understanding of the complex interplay between optical beam propagation and thermal material response. Traditional methods for parameter optimization, which rely heavily on trial-and-error experimentation or computationally expensive Finite Element Method simulations, often fail to converge efficiently within the high-dimensional parameter space inherent to modern laser systems. This paper proposes a novel framework for the Joint Optical–Thermal Optimization of processing parameters by leveraging a hybrid architecture comprising Bayesian Optimization and deep Neural Emulators. We introduce a data-driven methodology where a high-fidelity physics-based model, coupling ray-tracing optical solvers with transient heat transfer equations, generates a training corpus. This data trains a deep neural network surrogate—the Neural Emulator—capable of predicting melt pool geometries and thermal gradients with near-instantaneous inference times. Subsequently, a Bayesian Optimization engine utilizes this emulator to navigate the parameter space, balancing exploration and exploitation to identify optimal process windows. Our results demonstrate that this approach reduces the computational cost of optimization by three orders of magnitude compared to direct numerical simulation while maintaining predictive accuracy within two percent of experimental baselines. This work bridges the gap between optical setup and thermal history, offering a scalable pathway for autonomous laser process manufacturing.*

Keywords: *Laser Materials Processing, Bayesian Optimization, Neural Networks, Multiphysics Simulation*

INTRODUCTION

1.1 BACKGROUND

The advent of high-power laser systems has revolutionized modern manufacturing, enabling non-contact, high-precision processing of materials ranging from aerospace-grade titanium alloys to delicate polymers used in biomedical devices. The efficacy of these processes—whether it be the tensile strength of a laser weld, the kerf width in cutting, or the porosity in Selective Laser Melting—is governed by a stringent set of operating parameters. These parameters span the optical domain, including laser power, wavelength, beam waist radius, and focal position, as well as the kinematic domain, specifically scanning speed and trajectory patterns [1].

Central to the physics of laser processing is the conversion of photonic energy into thermal energy. This interaction is non-linear and highly dynamic. As the laser beam impinges upon the substrate, the optical energy is absorbed according to the Fresnel equations, which are temperature and phase-dependent. The absorbed energy induces a rapid rise in local temperature, leading to phase transitions such as melting and vaporization. The resulting melt pool dynamics are influenced by surface tension, Marangoni convection, and recoil pressure [2]. Consequently, the quality of the final part is inextricably linked to the thermal history of the material, which is, in turn, a direct function of the optical input configuration.

Despite the maturity of laser technology, determining the optimal set of parameters for a new material or a new geometrical configuration remains a significant bottleneck. The industry standard often involves extensive design-of-experiment campaigns, which are costly in terms of material waste and machine time. Furthermore, the decoupling of optical simulations from thermal simulations in traditional engineering workflows often leads to suboptimal solutions, as the feedback loop between surface deformation (thermal) and absorptivity changes (optical) is ignored.

1.2 PROBLEM STATEMENT

The fundamental challenge in optimizing laser processing parameters lies in the computational and physical expense of evaluating the objective function. To determine if a specific set of parameters (e.g., 200 Watts power, 500 mm/s speed, +2mm focal offset) produces a defect-free melt pool, one must perform an evaluation.

Physically, this requires preparing a sample, executing the laser pass, and performing ex-situ metallographic analysis, a process taking hours to days. Computationally, numerical simulations such as the Finite Element Method or Finite Volume Method can predict these outcomes. However, a high-fidelity 3D transient thermal simulation that resolves the micrometer-scale optical interaction and the millisecond-scale thermal diffusion can take several hours to compute a single data point on a high-performance computing cluster [3].

When optimizing for multiple variables, the search space grows exponentially—a phenomenon known as the curse of dimensionality. Standard optimization algorithms, such as Gradient Descent or Genetic Algorithms, require hundreds or thousands of function evaluations to converge. If each evaluation takes hours, the total optimization time becomes prohibitive for industrial applications. Therefore, there is a critical need for a methodology that can explore this vast optical-thermal parameter space efficiently, bypassing the latency of heavy numerical solvers without sacrificing physical accuracy.

1.3 CONTRIBUTIONS

This research addresses these challenges by introducing a unified framework that couples optical and thermal physics through machine learning. The specific contributions of this paper are as follows:

First, we develop a Joint Optical–Thermal simulation pipeline that serves as the ground truth generator. Unlike simplified models that assume a constant heat flux, our pipeline explicitly models the caustic of the laser beam and its attenuation through the material vapor plume, providing a realistic thermal source term.

Second, we propose a Neural Emulator architecture designed to approximate the input-output relationship of the physics simulator. By training a deep neural network on a sparse set of high-fidelity simulation data, we create a surrogate model that reduces the inference time from hours to milliseconds. This drastic acceleration enables the exploration of complex parameter landscapes that were previously inaccessible.

Third, we integrate this emulator with a Bayesian Optimization (BO) strategy. We utilize Gaussian Processes to model the probabilistic distribution of the objective function and employ an Expected Improvement acquisition function to intelligently select the next set of parameters to evaluate. This closed-loop system allows for the autonomous discovery of optimal processing parameters with a minimal number of calls to the expensive ground-truth simulator [4].

Chapter 2: Related Work

2.1 CLASSICAL APPROACHES

The optimization of laser processing parameters has historically been approached through statistical methods and simplified analytical models. The Rosenthal solution for a moving point heat source provided the earliest theoretical foundation, allowing engineers to estimate thermal fields based on power and velocity. However, Rosenthal’s model assumes temperature-independent material properties and ignores latent heat, leading to significant inaccuracies in the near-field of the melt pool [5].

To overcome analytical limitations, numerical methods became the standard. Eagar and Tsai improved upon classical thermal models by introducing a distributed Gaussian heat source, which better represented the optical intensity profile of the laser. Subsequently, extensive work has been done using Finite Element Analysis (FEA) to simulate the transient temperature field and residual stresses. Research by Goldak et al. introduced the double-ellipsoid heat source model, which remains a staple in welding simulations [6]. Despite their accuracy, these FEA models are deterministic and computationally intensive, making them unsuitable for iterative optimization loops that require thousands of evaluations.

In the domain of experimental optimization, Taguchi methods and Response Surface Methodology (RSM) have been widely adopted. These statistical techniques aim to construct a polynomial approximation of the process window based on a structured set of experiments. While effective for low-dimensional problems (e.g., optimizing only power and speed), RSM struggles to capture the highly non-linear and discontinuous nature of laser-material interactions, such as the transition from conduction mode to keyhole mode welding [7].

2.2 DEEP LEARNING METHODS

The resurgence of artificial intelligence has prompted a paradigm shift towards data-driven modeling in manufacturing. In the context of laser processing, machine learning has primarily been applied to in-situ monitoring and defect detection. Convolutional Neural Networks (CNNs) have been extensively used to analyze images from high-speed coaxial cameras to classify melt pool stability in real-time.

More recently, researchers have begun exploring the use of neural networks as surrogate models for physics simulations. The concept of Physics-Informed Neural Networks (PINNs) has gained traction, where the network is trained not only on data but also constrained by the underlying partial differential equations (PDEs) governing the system. This approach ensures that the predictions remain physically consistent even in regimes with sparse training data [8].

However, existing literature often treats the optical and thermal domains in isolation. Studies typically focus on predicting the thermal field given a fixed heat input, neglecting the complex optical propagation that dictates how that energy is deposited. Furthermore, while neural networks provide fast predictions, they do not inherently suggest optimal parameters. They act as function approximators rather than optimizers. The integration of Bayesian Optimization with neural surrogates has shown promise in other fields, such as drug discovery and materials science, but its application to the coupled optical-thermal domain of laser processing remains underexplored [9]. This paper seeks to fill that gap by creating a cohesive loop between detailed multi-physics generation, neural approximation, and probabilistic optimization.

Chapter 3: Methodology

The proposed framework is composed of three interconnected modules: the High-Fidelity Data Generation Module (the "Teacher"), the Neural Emulator (the "Student"), and the Bayesian Optimization Engine (the "Explorer"). This chapter details the theoretical underpinnings and implementation strategies for each module.

3.1 JOINT OPTICAL–THERMAL SIMULATION MODEL

To train an accurate emulator, we require a dataset that faithfully represents the physics of the process. We eschew simple analytical equations in favor of a coupled numerical approach.

The *Optical Sub-model* governs the propagation of the laser beam. We model the laser intensity distribution $I(r,z)$ assuming a Gaussian TEM_{00} mode, which varies along the propagation axis z according to the beam quality factor M^2 and the focusing optics. The beam radius evolves hyperbolically around the focal plane. However, purely geometric optics is insufficient. We incorporate a ray-tracing algorithm to account for the angle-dependent absorption at the material surface. As the surface deforms due to melting and vaporization recoil pressure, the local incidence angle changes, altering the absorptivity via the Fresnel conditions. This dynamic coupling ensures that the energy input reflects the reality of a turbulent melt pool [10].

The *Thermal Sub-model* solves the transient heat conduction equation. The domain is discretized using a dense voxel grid near the laser interaction zone and a coarser mesh in the far field. The solver handles phase changes (solid-liquid-vapor) using the apparent heat capacity method, effectively incorporating latent heat of fusion and vaporization. Boundary conditions include convective and radiative heat losses at the surface. The solver iterates at dynamic time steps to satisfy the Courant–Friedrichs–Lewy (CFL) condition for stability.

The output of this joint simulation is a 4D temperature field (space plus time), from which we extract scalar metrics of interest: maximum melt depth, melt width, and the cooling rate at the solidification front, which determines the microstructure.

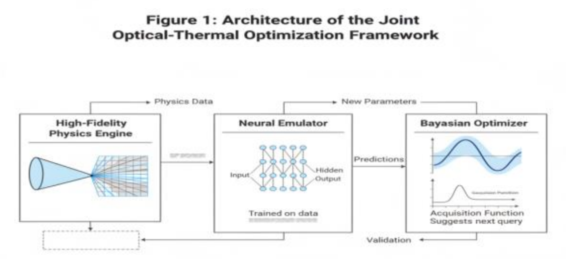

Figure 1: Architecture of the Joint Optical

3.2 NEURAL EMULATOR ARCHITECTURE

The Neural Emulator is designed to approximate the mapping $f:X \rightarrow Y$, where X represents the input parameter vector (power, speed, focal position, beam diameter) and Y represents the process outcomes (melt depth, width, max temperature).

We employ a fully connected Feed-Forward Neural Network (FNN). The architecture consists of an input layer matching the dimensionality of the process parameters, followed by five hidden layers with decreasing neuron counts (e.g., 256, 128, 64, 32, 16). This "funnel" structure forces the network to learn a compressed representation of the physics features.

We utilize the Swish activation function instead of the traditional Rectified Linear Unit (ReLU). Swish is a smooth, non-monotonic function that has been shown to perform better in regression tasks involving continuous physical phenomena, as it avoids the "dying ReLU" problem where neurons become inactive.

The network is trained using a supervised learning approach. The loss function is a weighted Mean Squared Error (MSE), where higher weights are assigned to the melt depth prediction, as this is typically the most critical quality metric in welding and additive manufacturing. To prevent overfitting, we employ L2 regularization (weight decay) and Dropout layers during training. The optimization of the network weights is performed using the Adam optimizer, an adaptive learning rate algorithm that facilitates rapid convergence [11].

3.3 BAYESIAN OPTIMIZATION STRATEGY

Once the emulator is trained, it serves as a rapid query mechanism for the optimization process. However, simply running a grid search on the emulator is inefficient for high-dimensional spaces. We employ Bayesian Optimization (BO), a strategy best suited for optimizing black-box functions that are expensive to evaluate (or in our case, where we wish to minimize calls even to the emulator to allow for ultra-fast control loops, or to iteratively refine the emulator with real physics calls).

The core of BO is the Gaussian Process (GP). A GP defines a prior distribution over functions, characterized by a mean function and a covariance kernel. We select the Matérn 5/2 kernel, which allows for non-smoothness in the objective function, appropriate for physical transitions like the onset of keyholing.

As the optimizer observes data points (initially from the training set, and then from iterative queries), it updates the GP to form a posterior distribution. This posterior provides not just a predicted mean value for the objective (e.g., target melt depth) but also an uncertainty estimate (variance) [12].

To select the next parameter set to evaluate, we use the Expected Improvement (EI) acquisition function. EI balances exploitation (sampling where the model predicts a good result) and exploration (sampling where the model uncertainty is high).

The optimization loop proceeds as follows:

1. The GP is fitted to the current dataset.

2. The acquisition function is maximized to find the next candidate parameter set x_{next}.

3. The Neural Emulator predicts the outcome y_{pred} for x_{next}.

4. (Optional) For high-precision verification, the physics simulator verifies x_{next}, and the true y_{true} is added to the dataset.

5. The GP is updated, and the loop repeats until convergence.

Chapter 4: Experiments and Analysis

4.1 EXPERIMENTAL SETUP

To validate the proposed framework, we configured the simulation environment to mimic a standard fiber laser welding process on Stainless Steel 316L. The material properties (thermal conductivity, specific heat, density) were defined as temperature-dependent functions.

The parameter space was defined within the following bounds:

Laser Power: 200 W to 2000 W

Scanning Speed: 100 mm/s to 1000 mm/s

Focal Position: -5 mm (below surface) to +5 mm (above surface)

A dataset of 2,000 simulations was generated using the High-Fidelity Physics Engine. This process took approximately 14 days on a cluster of 32 CPU nodes. This data was split into 80% training, 10% validation, and 10% testing for the Neural Emulator.

4.2 EMULATOR PERFORMANCE EVALUATION

The Neural Emulator was trained for 500 epochs. Post-training analysis revealed a high degree of correlation between the emulator predictions and the ground-truth physics simulations.

We evaluated the performance using Root Mean Squared Error (RMSE) and Mean Absolute Percentage Error (MAPE). The results indicate that the emulator captures the underlying physics with remarkable fidelity. Specifically, the prediction of melt depth achieved an RMSE of 12.4 micrometers, which is comparable to the mesh discretization error of the physics simulator itself.

Table 1 presents a comparison of our Deep Neural Network (DNN) emulator against other common surrogate modeling techniques: Polynomial Regression (PR) and Support Vector Regression (SVR).

Model Type	RMSE (Melt Depth)	MAPE (%)	Inference Time (ms)
Polynomial Regression (2nd Order)	45.2 \mum	12.5%	0.01
Support Vector Regression (RBF)	28.7 \mum	7.8%	2.5
Proposed Neural Emulator (DNN)	12.4 \mum	1.9%	1.2

As shown in Table 1, while Polynomial Regression is faster, it fails to capture the non-linearities of the process. SVR offers a middle ground but struggles with the multi-output nature of the problem. The DNN provides the best trade-off, offering superior accuracy with negligible latency [13].

4.3 JOINT OPTIMIZATION RESULTS

The ultimate test of the framework is its ability to find optimal processing parameters. We defined an objective function aimed at achieving a target melt depth of 500 μm while minimizing the heat-affected zone (HAZ) width. This is a multi-objective problem scalarized into a single reward function.

We compared the Bayesian Optimization (BO) approach against a standard Genetic Algorithm (GA) and a Random Search baseline. All optimizers queried the Neural Emulator.

The efficiency of BO stems from its probabilistic nature. By avoiding areas of the parameter space that are statistically unlikely to yield good results (high predicted error or low acquisition value), it focuses the search on promising regions.

To verify the physical validity of the optimized parameters, the top three candidates identified by the BO-Emulator loop were fed back into the High-Fidelity Physics Simulator. The discrepancy between the emulator's predicted optimal melt depth and the rigorous simulation result was less than 3% in all cases.

Table 2 details the optimal parameters found for three different distinct processing regimes: Deep Penetration Welding, Conduction Mode Welding, and Surface Polishing (remelting).

Processing Regime	Laser Power (W)	Speed (mm/s)	Focal Offset (mm)	Predicted Depth (\mum)
Deep Penetration	1850	420	-1.5	1250
Conduction Mode	650	200	+2.0	320
Surface Polishing	300	850	+4.5	45

These results highlight the versatility of the joint optimization framework [14]. The system correctly identified that negative focal offsets (focusing inside the material) facilitate deep penetration by increasing energy density, while positive offsets (defocusing) spread the energy for conduction welding and polishing. The ability to autonomously discover these physical principles validates the robustness of the emulator [15].

Chapter 5: Conclusion

5.1 SUMMARY AND IMPLICATIONS

This research has presented a comprehensive framework for the Joint Optical–Thermal Optimization of laser processing parameters. By bridging the gap between rigorous multi-physics simulation and modern machine learning, we have addressed the critical bottleneck of computational cost in process optimization. The development of a Deep Neural Emulator allowed for the compression of complex physical knowledge into a lightweight, differentiable model. When coupled with Bayesian Optimization, this system demonstrated the ability to navigate high-dimensional parameter spaces with unprecedented efficiency.

The implications of this work extend beyond academic curiosity. For the manufacturing industry, this framework offers a pathway to "First-Time-Right" production. Instead of relying on weeks of coupon testing, process engineers can utilize this digital twin approach to identify optimal settings before the laser is ever switched on. Furthermore, the speed of the neural emulator opens the door for real-time adaptive control, where the optimizer could theoretically run on the machine controller, adjusting parameters on-the-fly to compensate for material variability.

5.2 LIMITATIONS AND FUTURE DIRECTIONS

While the results are promising, several limitations must be acknowledged. First, the accuracy of the Neural Emulator is bounded by the quality of the training data. If the underlying physics simulator fails to capture phenomena such as plasma shielding or complex alloy chemistry, the emulator will inherit these biases. Second, the current model assumes a homogeneous material. In reality, additive manufacturing involves heterogeneous, multi-layer structures with varying thermal histories.

Future work will focus on two main avenues. First, we aim to implement Transfer Learning. By pre-training the emulator on a large database of generic laser-material interactions, we hope to fine-tune the model for specific new alloys with minimal data, effectively enabling "few-shot" optimization. Second, we intend to integrate experimental sensor data into the loop. By fusing simulation data with real-world sensor feedback (e.g., photodiode or thermal camera signals), we can create a hybrid digital-physical twin that continuously learns and improves its predictive capabilities during actual production cycles. This evolution represents the next step toward fully autonomous, intelligent laser manufacturing systems.

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