Bayesian optimization for enhanced plasma parameters in nanostructured plasma acceleration

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ABSTRACT

Nanostructures, particularly nanostructured plasmas facilitated by arrays of carbon nanotubes, could potentially offer a novel way for achieving ultra-high-density plasmas suitable for Laser Wakefield Acceleration (LWFA). Both the unique nanostructure of the plasma and the laser parameters significantly influence the wakefield properties, emphasizing the importance of optimizing structural parameters to attain high acceleration gradients. In this study, we employed the Particle-in-Cell (PIC) code EPOCH to simulate LWFA in nanostructured plasmas, systematically varying structure parameters to build a comprehensive database of configurations. Leveraging this database, we implemented Bayesian optimization using the Python module BoTorch to refine the parameters and maximize the acceleration gradient. Our results show the efficacy of Bayesian optimization in enhancing acceleration gradients within the modeled system, highlighting its utility in scenarios where precise functional behavior is challenging to ascertain. This approach holds significant promise for advancing laser-driven plasma acceleration technologies.

INTRODUCTION

Acceleration using solid-state nanostructured plasmas has recently attracted attention as a method of achieving ultra-high acceleration gradients, beam manipulation and gamma- or X-ray generation [1]. According to previous simulation studies [2, 3, 4], the excitation of high-density plasma wakefields in ionized solid-state structures using a finely tuned laser pulse could achieve

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electric field gradients in the order of $\mathrm{TV/m}$.

We study two setups for Laser Wakefield Acceleration (LWFA), where a single, short, high-intensity laser pulse excites a plasma wave. We need the laser pulse length to be in the order of the plasma wavelength, $L \simeq \lambda_p$. This ensures that the excitations created by the ponderomotive force are in phase with the pulse group velocity [5].

SIMULATION SETUP

Simulations were performed using the open-source PIC code EPOCH [6]. The investigated setups are shown in Fig. 1. The first one is a 2D multihollow periodic plasma, and the second one has a larger gap at the center. The plasma bands consist of preionized layers made of nanostructures, such as carbon nanotube bundles or carbon nanotube foam, which serve as media for generating high-density plasma.

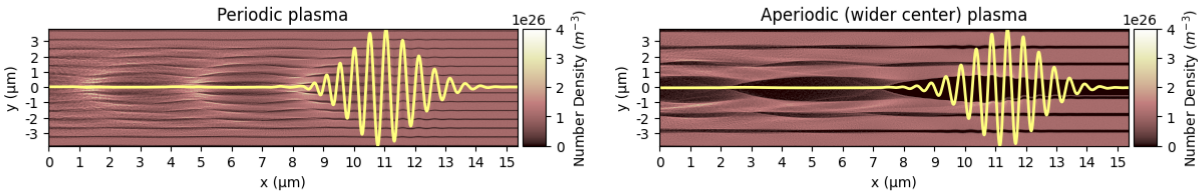

Figure 1: Nanometric structured periodic plasma (left) and nanometric structured aperiodic plasma with a wider center gap (right). The laser pulse crossing the structure is represented with a yellow solid line.

In Fig. 1 the laser pulse generates an excitation that injects plasma electrons into the center of the structure. This creates extremely high gradients, which can accelerate charged particles. The following laser parameters are considered: wavelength $\lambda_L = 500$ nm, intensity $I_L = 5 \times 10^{19}$ W/cm^2, pulse length $L = 0.5\ \lambda_p$ and phase $\phi = 0$.

In the first setup, we vary the width of the plasma bands, the gap between them, and the plasma density. In the second setup, we use the same parameters but also vary the gap in the center of the structure. Both simulations have a duration of 133.42 fs. We consider preionized electrons, assuming they are collisionless and without radiative effects.

The initial parameters define the domain over which the Bayesian optimization must find a solution. The maximum and minimum of each value define the limits of the domain. The following parameter ranges have been considered: plasma band width $\in [0.05, 1.5]$ µm; gap between bands $\in [0.05, 1.5]$ µm; plasma density $\in [0.5, 500] \times 10^{25}$ m^{-3}; and central gap (for the second setup) $\in [1, 3]$ µm. In total, we have performed over 200 simulations. The limiting parameters have been selected to encompass all the possible behaviours for the system, from structure breaking to pulse absortion. Somewhere in between we expect to find the optimal parameters.

BAYESIAN OPTIMIZATION

The Bayesian algorithm used in the optimization is found on the open-source Python module BoTorch, which is part of the PyTorch library [7].

The first setup maximizes the longitudinal wakefield amplitude and bubble size in the 2D plot of the electric field. The second setup maximizes the longitudinal and transverse wakefield amplitudes at the final step, as well as the frame-by-frame evolution of these two metrics.

After training, we need to run the simulations with the new parameters and assert if the metrics are better than the previous ones. Both models predict the candidates on a single iteration.

RESULTS

We produced six new candidates, three with the periodic setup and the other three with the aperiodic one, shown in Table 1.

Table 1: Key parameters for the best candidates in both setups

	Periodic setup			Aperiodic setup		
Parameter	P.1	P.2	P.3	A.1	A.2	A.3
Plasma band width (μm)	0.750	1.000	0.500	0.88	0.78	0.23
Gap between plasma bands (μm)	0.067	0.067	0.057	0.22	0.15	0.55
Central gap (μm)	-	-	-	1.00	1.00	1.47
Plasma density n_e (10^{26} m^{-3})	1.068	1.069	1.069	1.085	1.093	6.169
Longitudinal wakefield E_x (GV/m)	629.02	634.64	628.57	408.65	462.24	111.79
Transverse wakefield W_T (GV/m)	$\sim$250	$\sim$250	$\sim$250	27.291	10.365	2.403

The periodic candidates are quite similar, but the aperiodic ones have a wider range of behaviours, showing plasmonic excitations as a possible solution, e.g., case A.1 from Table 1. This result is very interesting, as it shows that the model is able to generalize.

As an example, Fig. 2 shows wakefields generated by different configurations.

Although the training was aimed at the blowout regime of LWFA, we found that the model generalized well to the linear plasmonic regime. This success is attributed to the use of superior metrics, which enhanced the model's capability.

Figure 2: Longitudinal electric wakefield on-axis (left) and transverse wakefield at $y = 1$ m off-set (right) for the candidates P.3 (top), and A.3 (bottom) from Table 1.

CONCLUSIONS

In these proceedings, we demonstrated that Bayesian optimization effectively optimizes parameters in PIC simulations of nanostructured solid-state plasmas. We trained two models with different metrics, both converging successfully. The second model required fewer simulations, highlighting the importance of metrics. Our results suggest broader applicability than initially expected, with potential for even greater versatility using improved metrics like beam emittance or particle acceleration thresholds. The current metrics focus on wakefields, so future development should include metrics for accelerated particles.

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