Modeling Needs for Structure Wakefield Accelerators

(Letter of Interest to Snowmass21, Computational Frontier)

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Abstract

Dielectric wakefield accelerators (DWFA), and more broadly structure-based wakefield accelerators (SWFA), are a candidate technology for a multi-TeV lepton collider. These systems promise orders of magnitude improvements in accelerating gradients over conventional RF-based accelerating technologies, thereby enabling access to TeV energies with a reduced footprint than, for example, the tens-of-kilometers required by the proposed Compact Linear Collider (CLIC). SWFA systems provide unique capabilities in comparison to their plasma-based counterparts, and the resulting demands for high fidelity modeling is equally unique. In addition to their sophisticated composition and geometry, the treatment of electromagnetic wave propagation at the interface of such boundaries requires careful consideration to avoid unphysical errors in field amplitude. This letter outlines some of the various device needs and corresponding modeling efforts being undertaken to support SWFAs, and highlights the challenges faced by the community in modeling the increasingly diverse array of complex experimental arrangements. Concerted development efforts will augment the development and testing of these novel accelerator systems.

1 Introduction

Modern SWFAs have made substantive strides towards higher gradients, smaller scale-lengths, and increased flexibility. Collinear SWFA schemes in which an intense electron bunch drives a trailing wakefield from which a witness beam can be accelerated, have demonstrated record GV/m-level gradients driven by ultrashort electron bunches within THz structures [1, 2]. For larger structures, operating at 200 GHz, peak fields of 320 MV/m have been observed, with peak surface fields of 500 MV/m [3]. The use of shaped drive-beams has enabled the demonstration of record transformer ratios in the generation accelerating fields [4].

As with other wakefield acceleration mechanisms, SWFAs enable sophisticated beam control, both by virtue of their size and through careful control of the structure's material properties and aperture. The manipulation of drive beam and structure characteristics has been shown to suppress unwanted mode excitation, with implications for witness beam stability during acceleration. For example, the use of elliptic drive beams has enabled the suppression of transverse wakes in planar structures [5]. New configurations, such as Bragg reflectors, photonic-band-gap, and woodpile structures, have been employed to better control fundamental frequency and higher order mode (HOM) characteristics [6, 7, 8]. Tapered structures

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have also been deployed to manipulate the phase velocity of the wakefield, enabling synchronous acceleration for improved longitudinal phase space control [9]. Additionally, novel metamaterials have been developed which enable reversed-Cherenkov wakefield radiation, permitting high gradient, GHz frequency acceleration from simple geometries [10]. Finally, the application of external fields to THz structures has enabled unprecedented longitudinal phase-space control of fs-scale, high brightness electron beams [11].

2 Current Modeling Paradigms

Simulation studies of SWFA systems vary in their demands and sophistication, owing to the variety of applications and associated figures of merit. For straightforward geometries, traditional particle-in-cell techniques enable self-consistent tracking of beam-driven wakefields with reasonable fidelity, but for more complex structures or optimization studies this is unfeasible. A common approach is to employ commercial codes to pre-calculate discrete wakefunctions for a fixed geometry and mesh, before integrating these values to obtain kicks for the particle beam of interest [9, 12]. An advantage of this approach is the ability to couple additional multiphysics considerations, for instance thermal coupling, electro-mechanical oscillations, and multipactor effort [13]. Such approaches have provided suitable dynamic predictions, but lack the fidelity in representing HOM excitation, or self-consistent effects from intense beam interactions. Moreover, they remain computationally expensive, as simulations must be repeated for different geometries and resolutions. In some cases, analytical solutions are preferred for extrapolating key figures of merit [14].

Modeling complex dielectric structures with finite-difference schemes can be challenging, as the discontinuity in the fields at surface interfaces can produce large errors in the fields, introducing global first-order errors and reducing simulation accuracy. Previous work to address this problem relied on an inverse dielectric matrix which had complex eigenvalues, leading to spurious exponential growth in the field amplitude [15, 16], while alternative algorithms have provided greater stability, but with inconsistent convergence scaling with grid resolution [17]. These difficulties present additional challenges for modeling layered structures, as resolution well below the layer thickness may be required to obtain accurate modeling of the structure modes. Other challenges include length- and time-scale disparities between the beam and structure, requiring trade-offs in grid resolution and fidelity to improve runtimes while minimizing finite differencing artifacts such as numerical Cherenkov radiation.

3 Prospective Developments

Modeling structure based wakefield accelerators for a high energy lepton collider requires high fidelity simulations for computing the electromagnetic modes of the structure. Short self-consistent electromagnetic simulations are useful for this purpose, but simulating over hundreds of thousands or millions of wavelengths of the structure fundamental mode for a full lepton collider. Thus, the electromagnetic modes should be extracted into wake functions to be used in reduced tracking models for faster design studies.

Higher fidelity electromagnetic models could be derived from first principles calculations based on the electromagnetic action. Early studies of variational algorithms for particle-in-cell simulations show a promising reduction in noise and smoother results due to the convolution integrals involved [18, 19]. This paradigm for algorithmic derivation has never been applied to dielectrics, and represents a research thrust of its own.

Modeling over hundreds of thousands to tens of millions of wavelengths of the fundamental structure is computationally expensive, and fully self-consistent electromagnetic PIC simulations should be reserved for final verification of a design. Improvements to PIC models, including higher-order Maxwell solvers and boosted frame techniques, have been applied with great success to plasma simulations, and could be extended to dielectric structures [20, 21]. Reduced models based on wake functions computed from these electromagnetic simulations would allow tracking code style studies of the beam dynamics at significantly reduced computational expense. For tractable geometries, semi-analytical solutions may help to overcome the computational costs of these and other fully self-consistent approaches. Furthermore, machine learning methods may provide means of generating fast-acting surrogate models in lieu of repeated high-fidelity simulations. Such approaches could then be used to determine a prospective final design, which could then be validated with more computationally expensive, but more physically complete, self-consistent electromagnetic PIC simulations of the final structure-based lepton collider. Continued development of exascale-capable libraries to support mesh refinement, load balancing, and field solvers will ameliorate these challenges.

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