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Towards Plasma-Driven Free-Electron Lasers

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Plasma-based accelerators are promising candidates to drive next-generation compact free-electron lasers (FEL) with unique X-ray properties. The correct modelling of the physics in the laser-plasma accelerator and of the FEL amplification from plasma-generated electron bunches thereby forms the basis for any application driven by these beams. Both problems are, however, extremely challenging. They heavily rely on computer simulations and, in fact, act as science drivers for the development of the latest generation of high-performance, highly parallel and efficient simulation codes. Here, we present our work towards a plasma-driven FEL, based on the particle-in-cell (PIC) codes VSIM and WARP, and the non-averaging 3D FEL code PUFFIN.

1 Introduction

Free-Electron Lasers (FEL) are essential tools for a broad scientific community to study the dynamic of matter on its natural length and time scale. The availability of today's large-scale facilities to users, however, is very limited. A new approach for a next-generation FEL is based on the concept of laser-plasma accelerators (LPA), promising extremely compact FEL setups, combined with unique features of the generated X-ray pulses.

The path towards a plasma-based FEL is extremely challenging. Foremost, the process of electron beam generation and acceleration within the plasma has to be controlled. As the processes within the plasma happen on μm length and femtosecond (fs) time scales, the whole field relies heavily on computer-simulations to (i) predict and study new acceleration techniques, (ii) design new experiments, and (iii) analyse experimental data. Correctly modelling the physics within a plasma accelerator, under the restriction of limited computational resources, is still an area of very active development within the community. In fact, it is one of the scientific drivers for the development of highly parallel, high-performance simulation codes. Following the laser-plasma interaction, the generated electron beam then emits X-ray pulses while propagating through the subsequent FEL undulator. Here, existing codes, that have been successfully used to model the physics of today's large-scale FEL facilities, are no longer sufficient to describe the physics involved. New codes are required, and in active development, as an essential tool to study the novel plasma-based FEL concepts.

Our project, *Towards Plasma-Driven Free-Electron Lasers*, covers crucial aspects of the development of a future plasma-based FEL. The electron beam quality, especially in

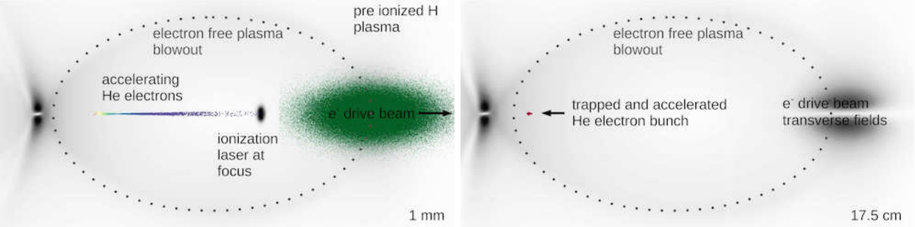

Figure 1. *Left:* Trojan Horse witness bunch generation. An electron beam (green particles) drives a plasma wakefield, represented by its field sum with up to 16 GV/m acceleration fields (gray). The high fields at the rear of the blowout are due to overshooting electrons, which were re-attracted to the drive beam axis. A strongly focused, short pulse laser (black) ionises neutral helium gas to generate free electrons in the wakefield (colour coded particles with 0-1 MeV energy). *Right:* The trapped witness has been accelerated to 1.1 GeV over a distance of 17.5 cm. Further parameters are 2.3 mm.mrad emittance, 10 pC charge, 2.1 kA peak current, and 1.2 % energy spread.

terms of energy spread and emittance, ultimately determines whether a beam is suitable to drive an FEL. It is therefore of utmost importance first, to generate high quality beams, and second, to maintain this quality throughout the acceleration section in the plasma and the subsequent transport to the FEL undulators.

In general, one can distinguish two different approaches in LPA: internal and external injection. In the former, an electron bunch is created inside the plasma from electrons that are pulled from the plasma background and directly accelerated within the same plasma target. In the latter, an external electron beam from a high quality source, such as a conventional accelerator, is injected into another plasma stage where it is further accelerated. In our project, we study both approaches. Electron beams studied in the two sub-projects are then imported into the new FEL simulation code, PUFFIN[1], that we develop and use to describe novel FEL schemes, based on plasma-generated electron beams.

2 Hybrid Systems and Underdense Plasma Photocathode

One path towards the generation of high-quality electron bunches is the underdense plasma photocathode (or “Trojan Horse” scheme). The central idea is to use an electron beam to drive a plasma wakefield, and employ a synchronised, strongly focused, short laser pulse to locally ionise additional electrons from a neutral high-ionisation-threshold background gas within the centre of the wakefield, see Fig. 1. We use the commercial PIC code VSIM to model this scheme, advance it conceptually, and to prepare and assist our granted beamtime at FACET[19] (experiment E-210). There, we will for the first time demonstrate the Trojan Horse concept experimentally.

In the Trojan Horse scheme, a cavity is generated by a high energy, high charge electron driver beam which expels electrons off axis, leaving a positive ion background and providing GV/m level accelerating fields – which is 2 to 3 orders of magnitude larger than in conventional RF cavities. The expelled electrons form a negatively charged electron boundary and become re-attracted towards the axis after one plasma wavelength, forming an electron-free cavity (also known as “blowout”). Electrons created from the synchronised laser pulse can be accelerated to high energies within the plasma wave, if the wakefield is strong enough to accelerate the electrons to relativistic energies within a length that is substantially smaller then one plasma wavelength. These electrons are then trapped at the rear of the plasma blowout – which is also moving with nearly the vacuum speed of light. The strong localisation of the electron release in combination with the low initial momentum of the electrons create high quality bunches of low emittance, that are then accelerated by the plasma wave. The scheme furthermore gives unprecedented control over the injection, and allows for tuning of charge and other important bunch parameters on a level of control hitherto only known from classical photocathodes.

Since the original publication[2] we could significantly advance this concept. A major requirement of electron beam driven accelerators is the need for a sufficiently strong electron beam driver, that, so far, requires a conventional large scale accelerator. We are therefore actively investigating laser-plasma accelerators as an alternative and more available source of suitable drive beams[3], and study methods to relax the requirements on the electron drive beam. This includes, for example, a plasma density downramp assisted trapping of electrons within the Trojan Horse scheme[5]. Here, the witness bunch electrons are ionised from the beginning of a plasma density downramp, which facilitates trapping, and thus allows for relaxed demands on the drive beam.

We could show that the demands on the driver electron beam quality in our Trojan Horse scheme are substantially lowered, compared for example to the requirements on bunch quality for FEL operation, and readily available by today's laser plasma accelerators[4]. We found, that the most crucial properties for FEL driver beams, energy spread and emittance, are quite unimportant for driving a plasma wakefield. Within the parameter range of today's laser-plasma accelerated bunches, an accelerated witness bunch is hardly affected by changing these properties of the drive beam. Other parameters like beam energy and current are more sensitive for a stable high gradient wakefield, and must not be beyond certain thresholds to guarantee stable acceleration, which is, however, a far easier task than generating small energy spread beams from a laser-plasma accelerator.

As another important achievement, we could propose a novel concept for witness bunch generation in beam driven plasma wakefield accelerators[17], which is easy to set up experimentally and can even help to implement the underdense photocathode mechanism. In this context, we studied the sources of dark current, which can significantly lower the quality of the witness bunch[18].

3 External Injection of Well-Defined Electron Bunches

A second concept to generate high-quality electron bunches, suitable for FEL operation, is based on well-defined electron beams from a conventional accelerator, that are injected into a subsequent plasma accelerator stage. By separating the tasks of electron beam generation, in the external electron source, from the actual acceleration, one could combine the advantages of both technologies: the extremely good control over the electron phase space in a conventional injector, and the huge accelerating field gradients in the plasma.

However, modelling these regimes requires mastering a new set of simulation technologies. External injection schemes typically operate with a significantly lower plasma density, compared to internal injection, which consequently lengthens the plasma target from only a few mm to a cm-scale. The significantly longer target can dramatically increase the computational costs of a PIC simulation. When modelling the problem in a

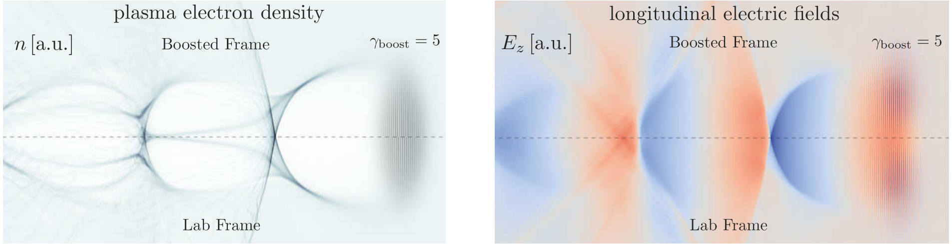

Figure 2. Comparison of the results of a 2D WARP simulation in a boosted frame ($\gamma_{\text{boost}} = 5$) with a reference simulation in the lab frame. The left panel shows the plasma electron density n, the right panel shows the longitudinal electric field E_z, both in arbitrary units. The upper half of the images corresponds to the back transformed results of the boosted frame simulation, whereas the results of the reference simulation are shown in the lower half.

Lorentz-boosted frame the plasma target gets contracted and it also propagates towards the laser. The number of timesteps and consequently the simulation runtime thereby can be reduced by up to a factor $2\gamma_{\text{boost}}^2$, where γ_{boost} is the Lorentz factor of the boosted frame. We are therefore actively contributing to the development of the open-source PIC code WARP, and its capabilities to operate in the Lorentz-boosted frame, which is essential for our work.

For example, to interpret the simulation data, it needs to be transformed from the boosted frame back to the laboratory frame. However, the space and time variables of the boosted and the lab frame are coupled. To create a dataset that covers the simulation space at one moment in lab time, snippets of data from many times and positions in the boosted frame need to be combined. We implemented efficient and performance optimised routines which sort and save the lab frame output on-the-fly in a boosted frame simulation. The agreement between the back-transformed data and a simulation in the lab frame is very good, as can be seen from Fig. 2.

With these techniques we study several crucial physics aspects of a plasma-based FEL: we proposed the adiabatic matching technique for plasma accelerators, as well as a plasma-based phase space diagnostics concept.

One severe challenge for external injection schemes arises from the focusing forces inside the plasma wakefield. In the plasma, the large accelerating fields are accompanied by strong transverse fields that focus the electron beam, and the externally injected beam needs to have a transverse beam size that is matched to these focusing fields. Otherwise, the beam size will oscillate around the matched beam size, like in a harmonic oscillator, which causes strong emittance growth[6]. However, this matched beam size is typically extremely small. In consequence, a very strong focusing optics before the plasma target is required to condition the beam to the plasma entrance, and also after the plasma stage, as the beam will also exit the plasma with a small beam size and consequently with a large divergence. This is not only challenging from a technological point of view, but also leads to emittance growth in the drift after the target[7].

This crucial issue can be tackled by properly designing the plasma target. Before and after the actual acceleration section a dedicated injection and extraction section is added to the target. There, the focusing forces are slowly increased or decreased and allow the bunch to adapt from vacuum to plasma and out into vacuum again[8]. The focusing forces are determined by the density profile and by the driver laser envelope, which need to be optimised in order to keep the sections short. For such optimisations extensive parameter scans in PIC simulations are inevitable.

Another challenge arises from the initially ultrashort few-fs bunches that are produced by laser-plasma accelerators. The bunch length is also a crucial parameter for external injection experiments. Since the accelerating field has a slope, different longitudinal slices of the bunch will experience a different accelerating field, which will increase energy spread. In order to minimise this effect, the bunches must be much shorter than one plasma wavelength. However, the measurement of bunch lengths and even current profiles with femtosecond resolution is extremely challenging.

In conventional accelerators, transverse deflecting structures are employed that are expensive, several meters long, and feature a resolution down to a few fs. For external injection experiments, we recently proposed to use a plasma target for the diagnostics of ultrashort electron beams[9], which promises a resolution of below 100 as, depending on the beam emittance and laser parameters. It does not require any additional instruments, as it employs the already installed driver laser. However, the method is sensitive to beam loading, which distorts the wakefield by the self-fields of the accelerated beam. These effects are only accurately represented in 3D PIC simulations, which are computationally demanding owing to high requirements on both memory and CPU performance.

4 FEL Simulations with PUFFIN

A key component in the design of FEL facilities is the use of numerical codes. Commonly used FEL codes like GENESIS[10] perform various approximations of the mathematical models describing the FEL interaction, such as the slowly varying envelope approximation and averaging of the electron motion over a cycle, which limit their applicability. As such, they are not well suited to simulate some advanced FEL concepts. Neither do these approximations allow proper simulation of electron beams typically produced by laser plasma accelerators, which have quickly varying currents and a large range of energies.

Considering this, the so-called unaveraged 3D FEL simulation code PUFFIN[1] has been developed, which is free of limiting assumptions. The advantage is an enhanced resolution, revealing new physics and enabling proper simulation of some advanced FEL concepts; the downside is the increased computational demand required to model this higher resolution. As such, it is required to run PUFFIN on HPC machines, utilising MPI, when in full 3D mode, and the availability of sufficient HPC resources is now a crucial prerequisite for the design of novel FEL schemes.

Within our project *Towards Laser-Plasma Driven Free-Electron Lasers*, we significantly enhanced the features of PUFFIN to handle some peculiarities, which are intrinsic to novel, plasma-based FEL schemes. PUFFIN previously solved the radiation diffraction in Fourier space, implying periodic boundary conditions, which were causing problems when, under certain conditions, the radiation was propagating significantly outside the boundaries of the model[11], for example in proposed demonstration schemes for a first plasma-FEL[12]. A first priority was therefore the implementation of absorbing boundary conditions, which have now been utilised in the transverse plane in a method similar to Ref. 13, see Fig. 3.

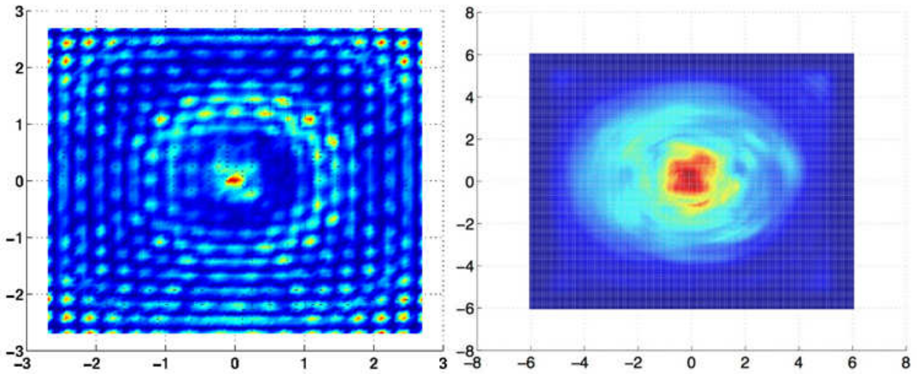

Figure 3. Typical output of the radiation field transverse plane (colour-coded intensity) in extreme diffraction regimes both before (left) and after (right) the implementation of absorbing boundary conditions. One can see a interference pattern before the boundaries were implemented, caused by the interference between the outgoing (towards the edges) emitted radiation and the incoming (from the edges) reflected radiation. This unphysical problem is mitigated by absorbing the radiation (right panel).

Another improvement over the originally presented code[1] is the inclusion of a 3D magnetic undulator field[20], that enables us to model realistic experiments. Previously, an artificial focusing channel was super-imposed on the 1D undulator field to approximate a so-called “natural focusing”; now this 3D focusing motion emerges naturally from the 3D magnetic undulator fields. In addition, various algorithmic improvements, such as a slightly modified field driving algorithm, which removes the need for a stiffness matrix (as was previously required and described in Ref. 1), and by paying careful attention to array storage, have reduced the run time by around 75 %.

These new features are crucial to study new FEL regimes, among which is a two-colour FEL scheme with wide frequency separation, as proposed in Ref. 14. In an FEL, the electron beam energy is usually resonant with only one radiated frequency. By switching the resonance condition between two widely separated, strongly non-harmonic frequencies in PUFFIN, the electron beam is shown to bunch at not only these frequencies, but the sum and difference frequencies, and the higher harmonics[14], see Fig. 4. A bunching at a given frequency means the beam will radiate and amplify at that frequency quickly if it is also resonant. This could be exploited in future FEL designs to quickly generate multiple additional colours in the FEL output. This result, involving such widely separated frequencies, cannot be obtained using averaged FEL codes, which are limited to simulating amplification within a narrow bandwidth around a defined central frequency (and the higher harmonics of this frequency). PUFFIN, being an unaveraged code, simulates the full radiation spectrum self-consistently.

Due to this higher resolution, PUFFIN is also ideally suited for simulating the radiation arising from fine structures in the electron pulse. Based on such structures in the bunch[15], we proposed in Ref. 16 a novel scheme that may improve the beam’s condition for lasing, or spontaneously produce high power, coherent radiation.

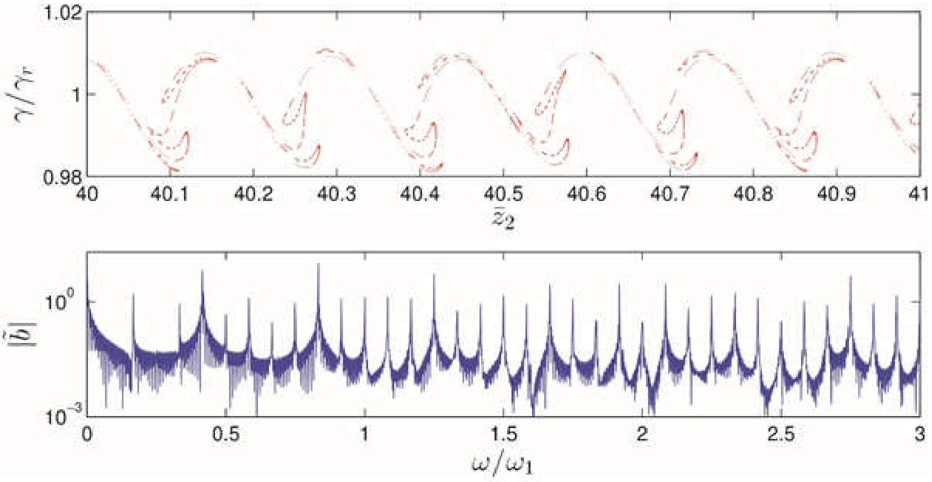

Figure 4. Electron beam phase space (top) and the electron beam bunching parameter as a function of frequency (bottom) at the end of our proposed 2 colour FEL scheme[14]. The beam phase space exhibits an oscillation at the shorter wavelength, which is “folded” into the oscillation at the longer wavelength. This results in the beam being bunched at not only these frequencies (the spikes in the bunching spectrum at frequencies 1 and 0.4), but also the sum and difference, and higher harmonics of these frequencies.

5 Concluding Remarks

Future plasma-based FELs would have an enormous impact on many scientific disciplines. The path towards a first successful realisation crucially requires advanced simulation codes, to model and study the new physics involved. To this end, we use a variety of codes, and we are specifically developing some of them to address physical problems, inherent to a plasma-based FEL. Over the past two years, we could show significant progress in addressing crucial aspects towards a future plasma-FEL, including enhanced beam quality from plasma accelerators, beam transport, and correct modelling of novel FEL schemes.

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