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Numerical Studies towards a Plasma-Driven Free-Electron Laser

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In a plasma accelerator, a laser or particle beam excites a plasma wave that can sustain orders of magnitude higher electric fields than the RF-cavities of conventional accelerators. These compact devices have the potential to drive next-generation free-electron lasers (FEL) of reduced size and cost. However, the highly sensitive FEL mechanism imposes strict requirements on the electron beam properties. So far, the quality of plasma accelerated beams cannot compete with that of conventional accelerators. Successfully driving the self-amplifying process demands the development of methods with increased control of the beam's phase space - in combination with novel FEL designs that leverage the unique features of the plasma accelerated beams. Demonstrating a plasma-driven FEL therefore heavily relies on theoretical studies and requires numerical models that correctly represent the physics involved under the restriction of limited computational resources. Here, we present our recent work towards a plasma-driven FEL, based on the particle-in-cell (PIC) code FBPIC, and the non-averaging 3D FEL code PUFFIN.

1 Introduction

Free-electron lasers (FEL) represent the latest generation of high-brightness light sources accessing, for the first time, matter and its dynamics on atomic time and lengths scales. Naturally, the demand for access to the currently existing FELs greatly exceeds the available beam-time, which is limited due to the high costs connected with large-scale facilities. To satisfy the demand from users, the accelerator physics community is developing concepts for the next-generation light sources, aiming for further improvements of currently accessible FELs in terms of facility costs (availability), as well as pulse length and synchronisation. One path towards increased availability for users (by decreasing facility size) and better time resolution for dynamic studies, are plasma-based accelerators as novel electron sources for FELs[1]. In a plasma wakefield accelerator a driver beam, either a laser pulse or energetic electron bunch, separates plasma electrons from the static ion background, thus creating a charge separation on the scale of the plasma wavelength (tens of μm), which is the origin of strong longitudinal and transverse electric fields. With accelerating gradients many orders of magnitude higher than in conventionally operated RF cavities, the required accelerator length can be reduced from few km to the laboratory-scale of a few meters. High energy electron beams in the GeV-level, with few percent energy spreads, low emittances and few-femtosecond bunch lengths, have been demonstrated experimentally. However, the quality of plasma-accelerated beams cannot yet compete with conventional accelerators. As FELs put stringent requirements on the electron beam properties, novel FEL designs and concepts to further improve the quality of plasma accelerated beams are required.

On this path towards a plasma-driven FEL, numerical studies play a crucial rule. Here, we present a selection of our recent theoretical work where we address several critical issues in a holistic approach. This includes novel concepts to improve the quality of plasma accelerated beams (Sec. 2), studies on the dynamics of the FEL process when driven with those beams (Sec. 3), as well as the development of numerical algorithms with improved accuracy (Sec. 4) and efficient simulation codes (Sec. 5) suitable to correctly model the complex plasma acceleration and FEL processes.

2 Electron Beam Quality Conservation in Laser-Plasma Accelerators

The common method to generate electron beams for acceleration within the plasma wave relies on injecting a small portion of electrons from the plasma background into the accelerating phase of the plasma wakefield. Although these self-injection methods are widely used, they can suffer from poor quality and stability. In addition to improving these plasma-injected electron beams by developing advanced methods to precisely control the injection mechanism, it is also possible to externally inject a high quality beam from a conventional accelerator that is further accelerated to high energies in the plasma wave. Especially in the case of external injection, but also in the case of self-injected beams, a major challenge is to conserve the initial beam quality of the electron bunch throughout its acceleration in the plasma.

We suggested several new concepts to preserve and diagnose the electron beam quality: We proposed the adiabatic matching technique[2] to maintain beam quality during extraction from plasma to the electron beam transport and a new method to diagnose the longitudinal beam profile with sub-fs resolution[3]. Recently, we developed a new method to eliminate the build-up of a linear energy chirp and thus limit the beam energy spread[4]. This so-called modulated plasma density scheme holds great promise to minimise the energy spread an electron beam acquires during acceleration in the plasma. By changing the plasma density, the phase of an electron bunch within a plasma wakefield can be adjusted, which allows to actively shape the accelerating fields acting on the bunch.

In the plasma wave, the sinusoidal accelerating (decelerating) electric wakefields are phase-shifted by a quarter plasma wavelength with respect to the transverse focusing (defocusing) wakefields. In the typical configuration, the position of the electron beam is constrained to the region where it experiences both, accelerating and focusing forces. At this phase, however, the positive slope of the accelerating field imprints a correlated energy spread onto the electron bunch. By periodically modulating the plasma density along the accelerating length, the electron beam can be shifted between phases of the wakefield with a positive and negative slope of the accelerating field, which effectively flattens the net accelerating gradient. Although this causes the bunch to oscillate between transversally focusing and defocusing regions, we showed that stable beam transport along the accelerator is still possible[4].

An example is shown in Fig. 1. The density is modulated by a factor of three on a mm-scale, which mitigates the build-up of a linearly correlated energy spread. The final projected energy spread in this example is reduced to 0.2% compared to 1% for a constant

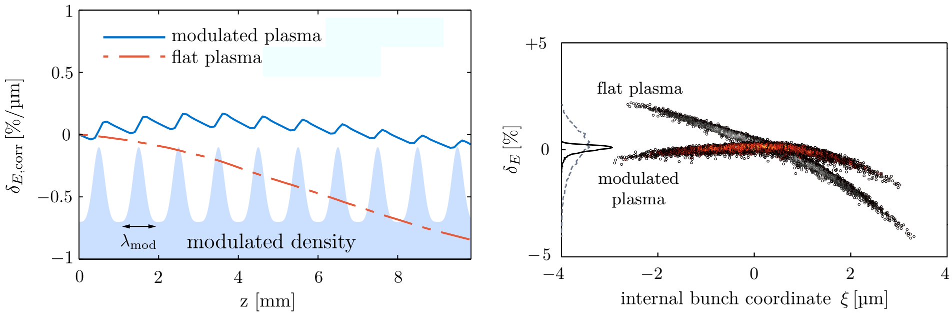

Figure 1. (left) Evolution of the correlated energy spread (chirp) $\delta_{E,\text{corr}} = \langle zE_{\text{kin}}\rangle/\langle z^2\rangle\bar{E}_{\text{kin}}$. The chirp evolution for the constant focusing reference case is indicated in red, while the blue line shows the chirp evolution using the modulated plasma density. The grey shaded area indicates the modulated plasma density profile. In the reference case the beam has accumulated a negative chirp with a final relative energy spread of 1%, while the chirp is compensated using a modulated plasma density with a final relative energy spread of 0.2%. (right) Electron beam phase space after the propagation through the plasma. Here, $\delta_E = \Delta E_{\text{kin}}/\bar{E}_{\text{kin}}$. Figures adapted from Brinkmann *et al.*[4].

density plasma. The proposed concept has great potential to be applied experimentally to significantly improve the beam quality of plasma accelerated bunches.

3 Effects of Strong Energy Correlations in Free-Electron Lasers

Despite the development of numerous techniques to improve the quality of plasma-accelerated beams, such as those described in the previous section, the plasma beams available today still suffer from an energy spread that is orders of magnitude higher than that of conventional accelerators. Nevertheless, as the plasma beams typically offer very short bunch lengths and high currents, it is possible to stretch the electron beam, thereby reducing its energy spread locally, while imprinting an energy chirp globally. This reduction in slice energy spread is essential to drive the FEL process, whereas the deleterious effects caused by the global chirp can usually be mitigated by tapering the undulator magnetic field[1]. However, the plasma-accelerated beams can possess a large enough energy chirp to show extra effects beyond the currently accepted theory[5]. The first is that the beam stretches as it propagates through the undulator, changing the lasing characteristics. The second is that the usual form of the taper used to compensate for the chirp must be reconsidered in more detail. An example of the implications of these effects on the FEL operation is shown in Fig. 2. It is important to consider these effects in the development of a free-electron laser using the beams from plasma accelerators.

4 Numerical Instabilities in Particle-In-Cell Codes

In order to experimentally realise a sensitive system like a plasma-driven FEL, theoretical investigations like the ones presented above are indispensable. However, due to the complexity of the physics involved, the interactions often cannot be described appropriately with analytical models. Therefore, numerical simulations are a vital tool in the fields of

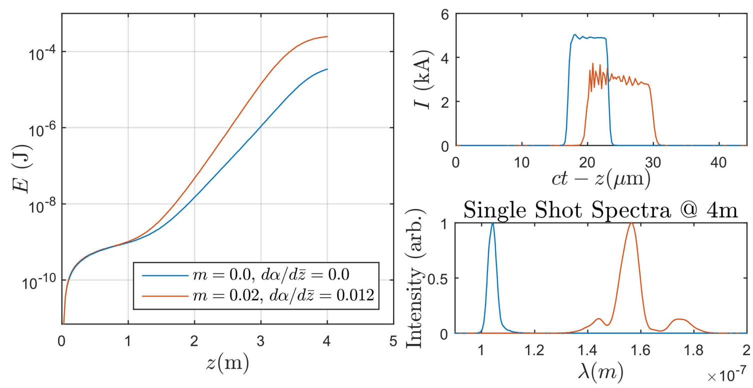

Figure 2. Effect of the large energy chirp on the lasing of a short electron beam. Blue lines - without chirp. Red lines - with chirp. Left plot: Radiated energy as a function of distance through the undulator. Top right: Final current. Bottom right: Spectral output. One can observe that for these parameters, the chirp results in the total radiated energy being higher than the unchirped case, but at a longer wavelength. Figure taken from Campbell *et al.*[5].

plasma acceleration and FEL physics. In plasma physics common tools are particle-in-cell codes. These codes work with a minimum of physical assumptions, but they can suffer from severe numerical instabilities. Their implications on the physical simulation results, as well as solutions to mitigate them, will be discussed in this section.

A particle-in-cell code models a physical system by representing its field and particles on a discrete grid and in a continuous phase space, respectively. It then propagates this system in time by iteratively and self-consistently solving the set of Lorentz' and Maxwell's equation describing its dynamics.

Common solvers impose approximations on the derivatives representing Maxwell's equations. This can unphysically alter the electromagnetic dispersion relation which leads to instabilities of the algorithm. An artifact resulting from the discrepancy between the physical and numerical speed of light is the so-called Numerical Cherenkov Radiation (NCR). Higher orders of this instability can occur when modelling plasmas drifting at relativistic velocities. The effect is then commonly referred to as Numerical Cherenkov Instability (NCI).

NCR is artificial radiation coherently emitted by charged particles propagating with the same velocity as the incorrectly modelled speed of light. It can be a dominant source of spurious beam quality degradation in terms of emittance and energy spread[6]. Due to the extreme sensitivity of the FEL process to these crucial beam parameters mitigation of NCR is inevitable.

As a result of their high spectral precision pseudo-spectral solvers[7] suppress NCR. However, due to the global nature of the Fourier transform used by these solvers they are unsuited for parallelisation of the computation by spatially decomposing the simulation box. The Arbitrary Order Pseudo-Spectral solver (PSAOTD) is an extension of these solvers. By representing Maxwell's equations with tunable precision, it can provide the needed locality for parallelisation and quasi-spectral accuracy in order to suppress NCR.

Fig. 3 shows the effect of NCR in a comparison of the infinite order Pseudo-Spectral

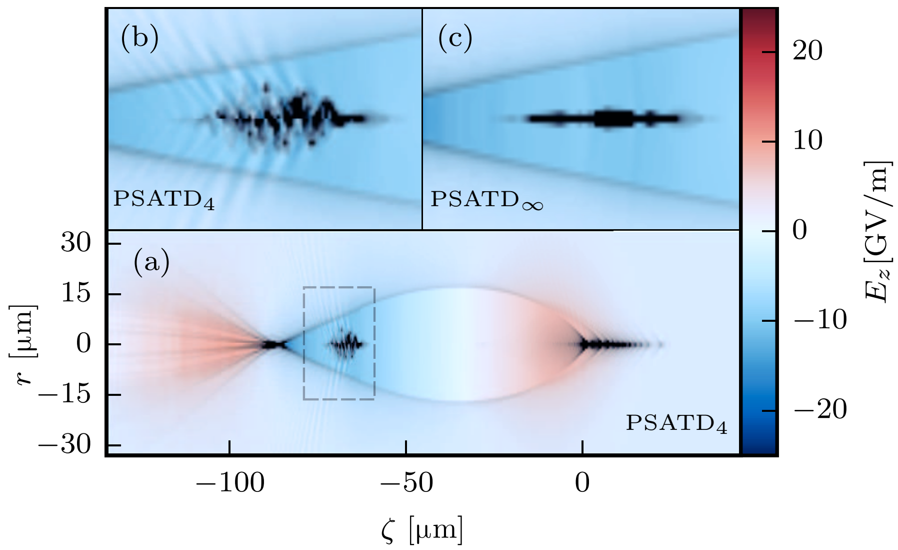

Figure 3. Electron beam quality degradation caused by Numerical Cherenkov Radiation (NCR). Particle-in-cell simulation of a beam driven plasma wakefield with a second electron bunch that is accelerated (a). In the case of a low-order solver (PSATD4) (b) the beam quality is degraded due to NCR - indicated by the high-frequency oscillations of the electromagnetic fields. In the case of an infinite-order spectral solver (c), the beam quality is preserved. Figure taken from Jalas *et al.*[6].

Analytical Time Domain ($PSATD_\infty$) and a low order PSAOTD solver. While NCR is still critical for very low solver orders, for typical parameters of plasma based accelerators we have found that already moderately high orders of these solvers are sufficient to suppress NCR. The PSAOTD solver allows to correctly model the physics of interest while also offering the locality needed for parallelisation[6].

Designing a plasma-based electron source suitable to drive a free-electron laser requires to conduct parameter studies and large-scale simulations of long plasmas. However, this is often unfeasible - or even impossible - due to the high computational costs of particle-in-cell simulations. One approach to drastically reduce the computational cost of PIC simulations is the so-called Lorentz-boosted frame method. It allows to speed up plasma acceleration simulations by orders of magnitude by transforming the physical quantities to an optimal frame of reference that co-propagates with the driver laser. In this Lorentz-boosted frame, the constraints on spatial resolution are reduced while significantly lowering the total interaction time. Thereby, the required amount of time steps is greatly reduced.

However, the occurrence of the Numerical Cherenkov Instability fundamentally limits the applicability of the Lorentz-boosted frame method. This instability occurs because the plasma is streaming at a relativistic velocity in a Lorentz-boosted frame simulation. As the plasma particles move with respect to the static, discrete field grid in the PIC code, numerical distortions and aliasing effects can lead to fast growing unphysical waves. So far, this instability could only be mitigated by introducing artificial numerical corrections

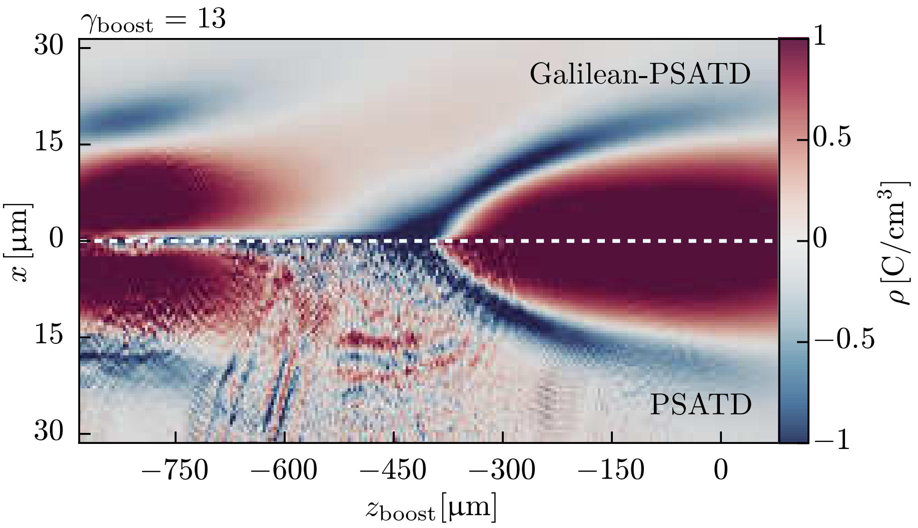

Figure 4. Density distribution of a plasma wave modelled in the Lorentz-boosted frame with a standard PSATD (bottom) and a Galilean-PSATD (top) solver. The Galilean-PSATD solver prevents the Numerical Cherenkov Instability. Figure taken from Kirchen *et al.*[8].

to a PIC algorithm that can potentially affect the physics. We developed a new method (embedded in the so-called Galilean-PSATD solver) that for the first time is intrinsically free of the Numerical Cherenkov Instability for drifting plasmas and that does not require any artificial numerical corrections[8,9].

Fig. 4 shows the direct comparison of a Lorentz-boosted frame simulation of a laser-plasma wave conducted with the standard PSATD and the Galilean-PSATD solver. While the former suffers from a fast growing instability, the Galilean-PSATD produces accurate results over the entire simulation length.

5 Development of Simulation Codes

The complex electromagnetic interaction within the plasma accelerator and the unique properties of plasma-accelerated beams with respect to modelling the FEL process put special requirements on the numerical tools used. Modelling those systems is computationally demanding. In this section we present the highly parallel codes FBPIC[10,11] and PUFFIN[12,13] that have been developed to accurately represent the physics involved, while employing efficient algorithms to decrease the computational costs.

FBPIC is a highly parallel particle-in-cell code to model plasma-based particle accelerators. Its uniqueness lies in the fact that it implements advanced algorithms that have been recently developed in the field of particle-in-cell modelling of plasmas. First, it solves the physical interaction in a quasi-cylindrical geometry, which greatly reduces the computational costs while retaining the three-dimensional properties of the physics involved. Second, it features a spectral electromagnetic field solver[7] implementing the concepts described in Sec. 4. When compared to traditional field solvers, these developments increase the accuracy of the physical results, while at the same time lead to a higher computational efficiency. The code is written in pure Python, while using the Numba Just-In-Time compiler to generate machine code with CPU multi-threading support and the possibility to execute on CUDA accelerated hardware. On a second level, the code is parallelised by domain decomposition with MPI, using the mpi4py package.

Both ultra-short pulse generation and plasma driven FEL research show an increasing demand for more advanced computational models of the FEL interaction. In particular, a 3D broad-bandwidth code that allows full evolution of the electron beam in 6D phase space is necessary for modelling such systems. PUFFIN is an unaveraged 3D FEL simulation code that solves the dynamics of an FEL without applying limitations like the slowly varying envelope approximation or averaging of the electron motion over one cycle. With its accuracy PUFFIN allows to model the effects that are particularly important when studying the FEL process with beams generated by plasma accelerators, such as the result in Fig. 2, which cannot be modelled in other commonly used FEL codes making more prohibitive assumptions. The code's high precision comes at the cost of computational demand. PUFFIN is parallelised with OpenMP and MPI in order run efficiently on large HPC systems.

In combination, these two codes allow to consistently model the transition from a laser pulse to an electron beam in the plasma and the transition of that electron beam to an X-ray pulse in a free-electron laser.

6 Concluding Remarks

We have presented approaches to solve some critical problems on the way towards plasma accelerator based FELs.

An intrinsic property of plasma accelerators is that the electron beams they produce acquire a correlated energy spread during the acceleration process. We showed a new method to compensate this energy correlation by using modulated plasmas. Further, we investigated the consequences of correlated energy spreads in FELs and showed how to optimise machine parameters to compensate them.

Theoretical studies on plasmas and FELs heavily rely on accurate numerical tools. For this, mitigation of numerical instabilities such as NCR and NCI is important. The use of specialised spectral solvers can suppress and even eliminate these numerical artifacts and allows simulations with high accuracy. We presented the codes PUFFIN and FBPIC which in combination are suited to model the complete physics of a plasma accelerator and a subsequent free-electron laser.

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