Angstrom wavelength FEL driven by 5 GeV LWFA beam with external injection

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Abstract. We report on simulation results relevant both for EuPRAXIA@SPARC LAB [1] and EuPRAXIA [2] showing how to boost a high brightness electron bunch, delivered by a conventional accelerator at 500 MeV, up to 5 GeV and more by external injection in a laser driven plasma wave. Beam slice quality is preserved along acceleration and the bunch is shown to be able to drive a Free Electron Laser at 1 Å wavelength. We also show two methods to evaluate global bunch parameters, one for energy spread, the other for emittance, allowing to exclude particles in halos and tails in a consistent way. Both methods are easily implemented in computational codes, are statistically robust and failure free.

1. Introduction

Laser WakeField Acceleration [3] is considered one of the most promising advanced acceleration techniques to reduce size and costs for electrons accelerators. This reduction would benefit large portions both of civil and scientific communities, allowing to bring electron beams enabled methodologies to university or hospital size facilities. To date, its potentialities have been extensively investigated worldwide by many laboratories [4, 5, 6, 7, 8, 9, 10, 11]. Possibly, one of the most sought after applications is the production of electromagnetic pulses by Free Electron Laser (FEL) [12], able to deliver high power photon bunches up to X-ray energies with at least partial transverse coherence [13]. At present, three projects [14, 15, 16] are trying to implement a LWFA driven FEL as test experiments; however, the interest in this topic is so high that the EuPRAXIA European design study has been founded and will be shortly delivered [2]. The EuPRAXIA@SPARC LAB project [1] is an Italian initiative, within the EuPRAXIA framework, aimed at fostering the candidature of INFN Frascati Labs to host EuPRAXIA infrastructure.

Among the many different proposed schemes for performing laser-plasma acceleration, most rely on the so called internal injection, where electrons to be accelerated originate from within the plasma, either from plasma background [17] or from specific gas mixtures where one of the species is somehow ionized in a (at least) partially controlled way [8]. However, the only scheme able to guarantee full control on the injected bunch is the external injection [18, 19, 20], where
the electron bunch is provided by a conventional accelerator and injected in plasma for energy boosting.

Following results published in [21], where it was shown by start-to-end simulations the possibility to drive an FEL in the water window wavelength [22] with a 1 GeV LWFA boosted electron bunch, this paper shows how those results can be extended to a 5 GeV energy beam to drive a Å wavelength FEL. The paper is structured as follows: in section 2 we briefly describe the simulation setup and justify parameter choice; in section Appendix A statistically robust methods for evaluating both emittance and energy spread, while in section 3 we show simulation results and assess the working point stability by varying many setup parameters. Section 4 reports on FEL performances while in section 5 we draw our conclusions.

2. Plasma acceleration simulation setup

External injection requires a bunch delivered by a conventional accelerator. We employ the beam used in [21] for the 1 GeV case, whose generation has been thoroughly reported in [23] and [24], so we only summarize its properties in Table 1. Notice that incoming bunch Twiss parameters are already tuned to perform a correct matching into plasma, while the bunch length is better represented by the FWHM than the rms since it has been longitudinally compressed by velocity bunching [25].

Table 1. Input beam parameters: energy $E$, transverse dimension $\sigma_{tr}$, length $L_{FWHM}$, charge $Q$, relative energy spread $dE/E$, normalized transverse emittance $\varepsilon_n$. The last quoted parameter, called chromatic length $L_c$, is described in [26].

| $E$ [MeV] | $\sigma_{tr}$ [$\mu$m] | $L_{FWHM}$ [fs] | $Q$ [pC] | $dE/E$ | $\varepsilon_n$ [$\text{mm-mrad}$] | $I_{peak}$ [kA] | $L_c$ [m] |
|-----------|-----------------|-----------------|--------|--------|-------------------------------|----------------|--------|
| 536.5     | 3               | 4.3             | 30     | $6.1 \times 10^{-4}$ | 0.44             | $\approx$3     | 36     |

The plasma target is assumed a discharge capillary with a length $L_{cap} = 50$ cm and a constant plasma density $n_0 = 10^{17}$ cm$^{-3}$, corresponding to a plasma wavelength $\lambda_p \approx 100 \mu$m ($k_p = 2\pi/\lambda_p \approx 6 \times 10^{-2}$ $\mu$m$^{-1}$). Input and output ramps are also considered, both with an exponential profile, i.e. $n(s) = n_0 \exp (\pm \Delta s/\lambda_c)$ with $s$ longitudinal coordinate, $n(s)$ local plasma density and $\Delta s$ the distance between the bunch and the capillary tips (the + sign apply for input ramp, - for output), whose characteristic length $\lambda_c$ is set at 5 mm: these ramps help both in matching the bunch into plasma [27, 28] and to extract it back to vacuum with minimal emittance degradation [29, 30, 31]. The 800 nm wavelength laser driver has an energy $E_l = 24.5$ J and is guided within the capillary at a nominal matched spot size $\sigma_l = 70 \mu$m [32]; pulse duration is $\tau = 112$ fs (FWHM) so that normalized laser strength results to be $a_0 = 1.15$, in order to excite a plasma wave in the quasi-linear regime. All plasma target and laser driver parameters are chosen so that $k_p \sigma_l > 1$, for maximizing the plasma wave velocity within plasma, thus increasing both dephasing ad pump depletion lengths (see [33] for example), together with a reasonably small ratio between bunch length and plasma wavelength in order to fit comfortably the bunch within a plasma bucket and reduce as much as possible the correlated energy spread. Further details can be found in [34].

Simulations are performed with the hybrid code QFluid [29], where cylindrical symmetry is assumed for the plasma response, while the electron bunch evolves in a fully 3D space. Simulation parameters are as follows: $k_p \Delta r \approx k_0 \Delta z \approx 0.1$, where $\Delta r$ and $\Delta z$ are transverse and longitudinal sampling, respectively, while the time step $\Delta t$ is set to $\omega_p \Delta t \approx 0.02$ ($\omega_p = ck_p$ with $c$ speed of light).
3. Beam dynamics simulation results and working point stability

Figure 1 reports properties of the final 5 GeV bunch and of its transport. In Figure 1 (a) the longitudinal phase space is depicted, showing a small signature of beam loading around the peak energy, i.e. where the peak of current is present. This signature originates two local minima for energy spread, as can be seen in Figure 1 (c), blue line, where the chromatic length exceeds 100 m. Notice that slice emittance value is different in the two minima positions (Figure 1 (c), red line). Final longitudinal phase space also shows two long energy tails, extending to $\approx 1$ GeV. They originate during acceleration, as shown in Figure 1 (d), green line, and are responsible for rms relative energy spread growth up to close 10%. Employing robust statistics to calculate relative energy spread returns an evolution which is much closer to the core part of the bunch (magenta line).

Figure 1. Top left. Final longitudinal phase space. Top right. Emittance evolution during acceleration: raw values of $x$ and $y$ emittances (red and light green, respectively) and the same parameters after a $7\sigma_{FIT}$ cut (magenta, green). Bottom left. Slice emittance properties: normalized emittance (red, left axis), chromatic length (green, left axis), energy spread (blue, left axis) and current (black, right axis). Bottom right. Energy spread evolution during acceleration: rms estimators (green) and robust estimators (magenta).

Figure 1 (b) shows evolution of normalized emittance both as raw data returned by QFluid (red and light green lines) and after a $7\sigma_{FIT}$ cut (magenta and green lines), as detailed in Appendix A. Spikes in raw data correspond to particles that are successively removed by simulation for going outside of simulation box; on contrary, cut data display a much smoother behavior whose value matches that of the slice with the largest current (Figure 1 (c), red line).
and imply an almost perfect matching to the plasma channel. The amount of charge lost during acceleration is about 0.5%, while the $7\sigma_{FTT}$ cut evaluation further removes another 1%.

**Table 2.** Tolerances allowing for a 10% variation of slice emittance, calculated on the largest current slice.

| $E$ [MeV] | $Q$ [pC] | $\sigma_z$ [\(\mu m\)] | $\alpha_T$ | $\beta_T$ [mm] | $\epsilon_n$ [mm – mrad] | $z_{b-L}$ [\(\mu m\)] |
|-----------|----------|---------------------------|------------|-----------------|-----------------------|------------------|
| 538$^{+44}_{-240}$ | 30$^{+5}_{-6}$ | 5.14$^{+3.27}_{-1.16}$ | 1.00$^{+0.45}_{-0.10}$ | 23.3$^{+3.4}_{-4.4}$ | 0.45$^{+0.05}_{-0.37}$ | 75.03$^{+1.40}_{-1.74}$ |

| $E_L$ [J] | $\tau$ [fs] | $Z_f$ [mm] | $n_p$ [$10^{17} \text{cm}^{-3}$] | $R_{ch}$ [\(\mu m\)] | $\lambda_c$ [mm] | $n_f$ [$10^{17} \text{cm}^{-3}$] |
|-----------|------------|-----------|-----------------|-----------------|------------|----------------|
| 24.5$^{+4.2}_{-1.5}$ | 113$^{+29}_{-27}$ | 0$^{+1}_{-6}$ | 1.0$^{+0.2}_{-0.1}$ | 70$^{+13}_{-21}$ | 2.50$^{+0.21}_{-0.07}$ | 1.00$^{+0.31}_{-0.30}$ |

We performed a sensitivity analysis of the working point against variations of many parameters pertaining the input electron bunch (energy $E$, charge $Q$, length $\sigma_z$, Twiss parameters $\alpha_T$ and $\beta_T$, normalized emittance $\epsilon_n$, distance from driver pulse $z_{b-L}$), input laser pulse (energy $E_L$, pulse length $\tau$, focus position $Z_f$) and plasma target parameters (plateau length $n_p$, laser matched spot size $R_{ch}$, input/output ramps characteristic length $\lambda_c$ and uniformity of plateau $n_f$). Parameters have been varied one at a time by ±10% with respect to nominal reference values, forming a set of three simulations for each parameter. Largest current slice normalized emittance and energy spread have been collected the three values fitted with a second order polynomial. This allowed to roughly estimate acceptable parameters variation for keeping emittance and energy spread within 10% of nominal reference value. Results are reported in Table 2 for emittance and in Table 3 for energy spread.

**Table 3.** Tolerances allowing for a 10% variation of slice energy spread, calculated on the largest current slice.

| $E$ [MeV] | $Q$ [pC] | $\sigma_z$ [\(\mu m\)] | $\alpha_T$ | $\beta_T$ [mm] | $\epsilon_n$ [mm – mrad] | $z_{b-L}$ [\(\mu m\)] |
|-----------|----------|---------------------------|------------|-----------------|-----------------------|------------------|
| 538$^{+13}_{-42}$ | 30$^{+1}_{-1}$ | 5.14$^{+0.28}_{-0.24}$ | 1.00$^{+0.25}_{-0.04}$ | 23.3$^{+0.9}_{-1.0}$ | 0.45$^{+0.00}_{-0.05}$ | 75.03$^{+0.40}_{-0.17}$ |

| $E_L$ [J] | $\tau$ [fs] | $Z_f$ [mm] | $n_p$ [$10^{17} \text{cm}^{-3}$] | $R_{ch}$ [\(\mu m\)] | $\lambda_c$ [mm] | $n_f$ [$10^{17} \text{cm}^{-3}$] |
|-----------|------------|-----------|-----------------|-----------------|------------|----------------|
| 24.5$^{+1.8}_{-0.2}$ | 113$^{+1}_{-8}$ | 0$^{+0}_{-2}$ | 1.0$^{+0.1}_{-0.0}$ | 70$^{+1}_{-2}$ | 2.50$^{+0.15}_{-0.02}$ | 1.00$^{+0.01}_{-0.09}$ |

It is evident, from reported results, how energy spread is much more sensitive than emittance to parameters variation. This comes as no surprise since small characteristic length scales and

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1 We assumed the acceleration stage had a linear growth/decrease from nominal value to $n_f$. 
large longitudinal fields, typical of plasma acceleration, both contribute to final energy spread value. Moreover, an unmatched bunch tends, in most situations, to reach an equilibrium where emittance value can still have an acceptable value, contrary to energy spreads than always grow indefinitely. The most critical parameter is the electron bunch injection phase $\varphi_b - L/a$; again, this was an expected result since time jitters are known to be critical for external injection schemes. A method for reducing them to sub fs level has been proposed in [35].

4. FEL simulations

In order to check if the accelerated beam is suitable for driving an FEL at the Angstrom wavelength level, we transported and matched the electron bunch to the undulator, following the procedure detailed in [26]. Afterwards, we performed a simulation using the code GENESIS 1.3 [36] and employing the reference beam as input file. We assumed an undulator wavelength $\lambda_u = 1.5$ cm and normalized strength $a_u = 0.8$. The lattice is formed by a 77 periods long undulator section followed by a $6\lambda_u$ long quadrupole, whose focusing gradient is $10$ T m$^{-1}$. The quadrupole is $2\lambda_u$ away from preceding and following undulator sections.

Simulation results are reported in Figure 2 where SASE growth of FEL signal along undulator is shown in (a), with bandwidth evolution in (c). The FEL radiation time structure and power spectrum are depicted in (b) and (d), respectively. Overall radiation parameters are as follows: radiation central wavelength is $\lambda_r = 0.11$ nm with a bandwidth of 0.15%, while total energy is $1.17 \mu$J, yielding $6.4 \times 10^8$ photons. The saturation length is around 80 m.

![Figure 2](image-url)
The unusual presence of two distinct radiation peaks, both in time and in energy, as clearly seen in Figure 2 (b) and (d), is due to the presence of two minima in slice energy spread (Figure 1 (c), blue line). In fact, normalized emittance slice value is almost constant if evaluated on the smaller radiation peak position and in between the two peaks, whereas energy spread increases from about $2.5 \times 10^{-4}$ to $5 \times 10^{-5}$ (still a small value). Considering that slice current also almost doubles from the first to the second position, we conclude that the two peaks structure must be ascribed to energy spread value. This demonstrates that energy spread is much more critical than emittance, whenever driving an Angstrom wavelength level FEL is the goal of plasma based accelerated bunches.

5. Conclusions
In this paper we reported numerical simulations supporting the possibility to drive an FEL at Angstrom wavelength by an electron beam whose energy has been increased from 500 MeV to 5 GeV by LWFA. We also described a procedure to evaluate core beam parameters which is statistically robust and can be easily implemented with failure free numerical routines. From an unexpected feature of FEL radiation, we came to the conclusion that slice energy spread value is much more critical than emittance for driving hard FEL radiation, so that much more efforts should be put on improving this parameter.

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Appendix A. Robust emittance and energy spread evaluation
Electron beams coming from plasma often display annoying features like halo formation, lost particles, tail elongation in longitudinal phase space, etc., that, although comprising a rather small fraction of total charge, may prevent a sound evaluation of global beam properties, namely emittance and/or energy spread, returning unreliably high rms values. From a statistical point of view, the problem arises because rms estimators are not statistically robust (see [37], for example).

Externally injected bunches suffer even more from cited problems since injection may involve loss of particles from accelerating bucket that may eventually be re-captured in subsequent plasma oscillations: simulation codes based on a discretization of the simulation volume (i.e. the simulation box) can easily identify and remove particles reaching or crossing simulation box boundaries but those somehow remaining in the box require more complex methods to be correctly spotted. Procedures candidate for sound parameters evaluation should possess four desirable properties:

(i) be statistically robust;

(ii) return a value that can easily be converted in an equivalent rms value; this requirement stems from allowing the possibility to appeal to the “equivalent Gaussian beam” [27] for operational reasons (e.g. matching in a transport channel). Moreover, comparisons between different procedures can benefit from a standard, widespread and accepted estimator;

(iii) be failure free, meaning the procedure always returns a numerical value;

(iv) allow for an easy and efficient implementation in codes and/or control systems.

Considering the stated desirable properties, we decided to evaluate energy employing the median (henceforth designed by an over bar $\bar{\cdot}$), in place of the mean $<E>$, and the energy spread with Median Absolute Deviation, $MAD(.)$ [37], replacing the rms $\sigma_E$, which are known to be robust estimators, there exist the easy conversion $\sigma \approx 1.4826 \, MAD(.)$, always return a value
Figure A1. Left: spectrum of the 5.3 GeV plasma boosted bunch presented in section 3 (blue line), at the end of the transport. Right: a zoom of the peak area. In red are visualized position, extent and values for standard estimators, while in dark green are robust estimators.

and, although not computationally very efficient, involving vector sorting, is easy to implement. As an example, Figure A1 (a) reports a typical spectrum returned by our simulations. A sharp peak around 5.3 GeV and long energy tail, extending down to \( \approx 1 \text{ GeV} \), are present; Figure A1 (b) shows a zoom of the peak area with position, extent and values of \( \langle E \rangle \), \( \sigma_E \) in red and of \( \bar{E} \) and \( \text{MAD}(E) \) in dark green. It is evident how robust estimators return values that represent the beam core in a much more fitting way.

Transverse parameters, in particular emittance, may be also retrieved by replacing rms with

Figure A2. Left: distribution of \( x \) values for the bunch presented in section 3 (blue dots), at the end of the transport and its fitting Gaussian (red line). In green, the \( \sigma_{\text{FIT}} \) is depicted. Right: value of \( \sigma_x \) (cyan line, left axis), \( \sigma_{px} \) (green line, left axis), \( \varepsilon_{nx} \) (magenta line, left axis) and fraction of cut charge (black line, right axis) as a function of \( n_{\text{cut}} \). Note that the abscissa axis has a break.
robust estimators. However, since it is frequent to estimate emittance by cutting a determined amount of charge (e.g. 90% emittance) we decided to apply a different method that can realize an effective charge cut. A procedure has been defined as follows: first, a reasonable binning of the quantity under study (say, \( x \)) is performed; reasonable means that the resulting profile does not wash out details nor it is affected, around the peak, by significant noise. Second, the profile is fitted by a Gaussian, whose variance is \( \sigma_{\text{FIT}} \). Third, all charge outside a length \( L_{\text{cut}} = n_{\text{cut}} \sigma_{\text{FIT}} \) from the Gaussian peak is removed; \( n_{\text{cut}} \) defines the cut extent, so that it is possible either to set a fixed value of \( n_{\text{cut}} \), allowing for a variable charge cut to be performed or set the amount of charge to be cut and retrieving the corresponding \( n_{\text{cut}} \) value. For operational ease, we used the first option. Finally, the procedure fourth step requires to calculate \( \sigma_x \) without the cut Figure A2 (a) shows a zoom of the peak area reporting the performed \( x \) binning (blue dots), the Gaussian fit (red line) and a visualization of the retrieved \( \sigma_{\text{FIT}} \) estimator; the binning itself extends both for positive and negative \( x \) values to \( \approx 100 \mu m \). Notice that the fitting Gaussian does not need to perfectly reproduce the peak height since the relevant parameter to be retrieved is peak width. Figure A2 (b) reports on variation of transverse \( \sigma_x \) (cyan line), \( \sigma_{\text{px}} \) (green line) and \( \varepsilon_{nx} \) (magenta line) parameters as a function of \( n_{\text{cut}} \). The percentage of cut charge is also reported (black line). This last parameter stabilizes to values close to, or below, 1% for \( n_{\text{cut}} > 3 \), while the former ones flatten out for \( n_{\text{cut}} > 4 \) and slowly grow up to a value larger than 40. The conclusion, valid in all situations considered, is that a value \( 5 \leq n_{\text{cut}} \leq 10 \) represents a good choice for this parameter. A further indication this choice is sensible comes from recognizing that the returned emittance value is very close to the largest current slice emittance value (Figure 1 (c)).

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