Stability of elliptical self-modulating long proton bunches in plasma wakefields

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Abstract. The AWAKE experiment at CERN recently demonstrated the world’s first acceleration of electrons in a proton-driven plasma wakefield accelerator. Such accelerators show great promise for a new generation of linear e-p colliders using 1-10 GV/m accelerating fields. Efficiently driving a wakefield requires 100-fold self-modulation of the 12cm Super Proton Synchrotron (SPS) proton bunch using a plasma-driven process which must be carefully controlled to saturation. Previous works have modelled this process assuming azimuthal symmetry of the transverse spatial and momentum profiles. In this work, 3D particle-in-cell (PIC) simulations with the code QuickPIC are used to model the self-modulation of non-round bunches. We find that asymmetry in the initial seed wakefield leads to the formation of highly asymmetric microbunches which evolve incoherently along the symmetry axes of the initial bunch profile. However, the resonantly-driven accelerating wakefield is highly stable to both focused and astigmatic non-round bunches.

1. Introduction
Proton-driven plasma wakefield acceleration (PWFA) has been demonstrated [1] as a solution to energy depletion of electron or laser drivers in long plasma channels suitable for accelerating bunches for generation of PWFA-based colliders for high energy physics research. However, available high-energy-content bunches, such as those from the Super Proton Synchrotron (SPS) used in the AWAKE experiment are too long by up to two orders of magnitude to efficiently drive a wakefield in a sufficiently dense plasma channel. Therefore, AWAKE relies on the seeded self-modulation (SSM) of the long SPS proton bunch within a plasma channel due to an initial, weak ‘seed’ wakefield (see figure 1). The seed is generated by co-propagating a laser pulse within the Gaussian proton bunch, close to its longitudinal midpoint, which excites an ionising front in the rubidium vapour channel. This causes an effective sharp-leading-edge bunch profile to be seen by the plasma, leading to weak excitation of a Langmuir plasma wave and periodic focusing and defocusing along the portion of the bunch that follows. If the resultant microbunch train is correctly longitudinally spaced, it can resonantly drive a wakefield of increasing amplitude along its length, which can be exploited for acceleration of other bunches behind the train.

Previous works have modelled the growth [2], phase [3] and saturation [4] characteristics of the non-linear SSM process, which must be carefully controlled to ensure efficiently arranged microbunches. While SSM has been shown to be highly sensitive to bunch parameters such
Figure 1. Schematic of seeded self-modulation (SSM). A long proton bunch (a), with a co-propagating ionising laser pulse generating an effective sharp-edged longitudinal profile, generates a seed wakefield with periodic focusing (vertical arrows), which leads to (b) the formation of a periodic microbunch train that resonantly drives a plasma wakefield suitable for high-gradient acceleration (horizontal arrows).

as transverse emittance and spot size [5] such works have almost consistently considered transversely round bunches or the effect of longitudinally varying centroid offsets leading to bunch hosing [6][7]. Here we present results from 3D particle-in-cell (PIC) simulations to investigate the SSM of bunches with perturbations of 2-fold rotational symmetry to their initial transverse spatial and momentum profile, and the effect on the resultant microbunch train and resonantly driven wakefields.

2. Simulation Parameters
Numerical simulations of the interaction of long proton bunches with similar parameters to the SPS bunches were performed using the 3D quasi-static PIC code QuickPIC [8]. Using a quasi-static simulation allows speedup of up to 3 orders of magnitude compared to a fully electromagnetic PIC simulation, under the approximation that the evolution timescale of the beam (and hence its wakefield) with respect to its propagation, is much slower than the time required to propagate over one length of the moving simulation window. Below we outline the baseline parameters, which were perturbed over multiple parameter scans. AWAKE baseline parameters are given in square brackets for comparison where different. Plasma of density $n_p = 2 \times 10^{14} \text{ cm}^{-3}$ [$10^{14-15} \text{ cm}^{-3}$] was used, corresponding to a skin-depth of $c/\omega_p = 0.373$ mm, where $c$ is the speed of light and the plasma frequency $\omega_p = 8.04 \times 10^{11} \text{ rad/s}$. For the baseline case, we take focused bunches with $\sigma_{xx} = \sigma_{yy} = 0$. In order to examine the physics of the modulation process the longitudinal profile was chosen to be flat-top with a leading edge of a sharp linear rise up to a nominal round-bunch baseline density of $n_{b0} = 0.01n_p$ [AWAKE bunch has half-Gaussian tail instead of uniform profile, with $\sigma_z = 12 \text{ cm}$ and $3 \times 10^{11}$ protons, giving peak $n_{b0} = 0.04n_p$ for the simulated $n_p$]. Where the initial bunches were asymmetrically compressed from a round shape with $\sigma_x = \sigma_y = 0.2 \text{ mm}$, $0.53 c/\omega_p$ (where $\sigma_x$ and $\sigma_y$ are the initial rms sizes of the bunch), $n_{b0}$ was scaled so as to conserve total bunch charge within parameter scans. Likewise, the transverse velocity spreads, $\sigma_{x'}$ and $\sigma_{y'}$, were scaled to preserve equal $x$ and $y$ normalised emittances of $3.5 \text{ mm mrad}$. The simulations were performed with 3D
Cartesian grids $x \times y \times \xi$ of $256 \times 256 \times 4096$ cells, spanning physical dimensions of $12 \times 12 \times 130$ $(c/\omega_p)^3$, where $\xi = ct - z$ is a co-propagating coordinate backward along the bunch axis, zeroed at the seed point $2 c/\omega_p$ from the leading edge of the simulation window. At this plasma density, this allows simulation of 20 microbunches within the simulation window [up to $\sim 100$ bunches from AWAKE beam]. The lower finite radius of the AWAKE plasma channel [$> 1$ mm $\sim 3 c/\omega_p$] was not considered. For simplicity, bunches were initialised with an energy of 400 GeV with no longitudinal momentum spread [0.03%], which is sufficiently high to allow quasi-static simulation. We further define the transverse aspect ratio at the plasma entrance, $a = \min(\sigma_x/\sigma_y, \sigma_y/\sigma_x)$, and the natural electric field $E_0 = m_e c \omega_p / e$ where $m_e$ and $e$ are the electron mass and fundamental charge, respectively.

### 3. Bunch Evolution

#### 3.1. Microbunch formation

The presence of higher order azimuthal modes in the initial transverse bunch charge distribution causes excitation of seed wakefields with azimuthal modes of equivalent orders as per linear plasma wakefield theory [6]. For an elliptical profile (with a quadratic dependence in $x$ and $y$), these contain contributions with rotation symmetry order $m = 2n \forall n \in \mathbb{Z}^+$, but under weakly non-linear evolution, will continue to be dominated by the strongest modes in the initial bunch profile, $m \lesssim 8$. As they drive the bunch modulation, the presence of these modes leads to strongly azimuthally varying transverse profiles of the formed microbunches. Note that the overall rotational symmetry will always be of order $\min(m)$. Figure 2 shows the transverse density distribution of a typical defocusing region (a) and microbunch (b) after the SSM has saturated. The distribution in the microbunch contains strong features aligned with the symmetry axes of the initial bunch and continues to evolve in asymmetric shapes. The ‘halo’ around the microbunch is a result of the phase shift of the focusing wakefield during the initial SSM growth phase [4] and is an artifact of a defocusing field present earlier at this position. Note that the defocused protons in (a), and those around the microbunch in (b), have relatively low azimuthal variation.

#### 3.2. Particle distribution

The asymmetry of the shape of the transverse wakefield in $x$ and $y$ leads to dephasing between oscillations in those directions of near-axis protons that form the microbunches. Figure 3 shows the $x$ and $y$ momentum distributions along the bunch axis, $\xi$, of a randomly sampled subset of simulated bunch particles after 3 m of propagation in plasma of an elliptical $a = 0.8$ bunch with $\sigma_y = \sigma_x/a = 0.53 c/\omega_p$. The frequency mismatch leads to a relative $\xi$-dependent phase shift between the $x$- and $y$- momentum distributions of the bunch, corresponding to asynchronous bunch motion along those directions. Figure 4 shows the normalised ratio of amplitudes of the
Figure 3. Momentum distribution of randomly sampled subset of simulation particles in $x$ and $y$ directions of an $a = \sigma_x / \sigma_y = 0.8$ bunch within after 7 m of propagation to the left.

Figure 4. Ratio of sum of azimuthal Fourier amplitudes of asymmetric $m = 2$ and 4 modes to the symmetric mode of the bunch transverse profile. The initial aspect ratio is $a = 0.8$, slices in $\xi$ along the bunch are at the simulation resolution and the bunch propagates to the left.

$m = 2$ and $m = 4$ Fourier modes to the $m = 0$ one, at each $\xi$-slice in the bunch. It is calculated as $A_{2,4;0} = (|F_2| + |F_4|)/|F_0|$ where the $F_m$ are the complex amplitudes at $m$ of the $r$-integrated azimuthal Fourier transform (FFT) of the transverse bunch charge distribution at each slice. The amplitudes in higher $m$ modes were found to be either negligible and, for $m > 8$, also insufficiently resolved by the discrete FFT. It is seen that the asymmetry is modulated nearly monochromatically with period $\approx 2\pi / k_p$ in $\xi$ in the linear-growth phase (1 m into plasma) [4] of the SSM. Note that in this phase, for sufficiently high $\xi$, there are regions where asymmetry of the profile is being reduced and correspond to initial defocusing regions of the seed wakefield. As the power in the asymmetric modes approaches that of the symmetric one (e.g. $\xi \rightarrow 25^- c / \omega_p$ at 3 m into plasma), the $\xi$ variation develops higher harmonics, presumably due to an onset of non-linear evolution of the bunch profile, and the acquired roundness is removed.

4. Wakefield Excitation

4.1. Focused bunches

The near-axis longitudinal electric field, $E_z$ is a useful measure of the acceleration gradient available to a narrow witness bunch, such as is the case in AWAKE [9]. Figure 5 compares the evolution of the on-axis $E_z$ with propagation distance over the bunch length for $a = 1$ and $a = 0.4$. The phase evolution and development is qualitatively similar despite the highly asymmetric microbunch shapes, which is likely due to charge containment within the transverse scale length of the narrow-bunch wakefield, $\sigma_x, \sigma_y \ll k_p^{-1}$. Figure 6 shows the time-evolution of $E_z$ for varying aspect ratio of the initial bunch, achieved by unidirectional, charge-preserving compression along the $x$ axis. Although the near invariance of the amplitude of maximum $E_z$
reached reflects phase stability of the resonant wakefield, its position along the plasma channel is seen to be sensitive to the aspect ratio, which may be a consequence an $a$-dependent initial exponential growth rate for the SSM.

**Figure 5.** Variation of the on-axis longitudinal electric field, $E_z$, along $\xi$ with propagation distance for focused bunches with (a) $a = 1$ and (b) $a = 0.4$.

**Figure 6.** Variation of the maximum on-axis longitudinal electric field, $E_z$, with propagation distance, within $\xi < 128 \ c/\omega_p$, for focused bunches with different $a$.

**Figure 7.** Variation of the maximum longitudinal electric field, $E_z$ within the simulation window, $0 < \xi < 128 \ c/\omega_p$, with propagation distance for bunches of different $a$ achieved by (b) under- and (d) over-focused bunches in $x$. The diagrams (a) and (c) illustrate the offset of the beta function in $x$ relative to that in $y$. 
4.2. Astigmatic bunches
A simple method to realise a transverse aspect ratio from a round baseline is to use an asymmetric final focus, leading to an astigmatic bunch. Here we use a modification to QuickPIC-OpenSource to initialise unequal aspect ratio due to such an offset in $x$-focus position, with a perturbation to the baseline, $\sigma_{xx'} > 0$ keeping the $x$-emittance, bunch charge and $y$-parameters unchanged. Figure 7 compares the $E_z$ evolution of such underfocused (a, b) and overfocused (c, d) bunches of peak density $n_b = 0.01n_p$, with longitudinally offset beta functions leading up to the plasma entrance. It is found that here the maximum $E_z$ is achieved later for $a < 1$ (as opposed to earlier for focused bunches), even though its maximum amplitude is once again only weakly sensitive to $a$. The evolution of $E_z$ is also less smooth in the over-focused case, likely due to the diverging initial spatial distribution.

5. Conclusions
We have used the particle-in-cell code QuickPIC to investigate the seeded self-modulation (SSM) of a long proton bunch of transverse profile with 2-fold rotational symmetry. It was found that the asymmetry of the bunch is modulated periodically by the seed wakefield during the initial linear growth phase. As the modulation progresses, the resultant microbunches acquire strong azimuthal variation in their transverse profiles as a consequence of a relative phase shift along the bunch axis of the $x$ and $y$ momentum distributions of the bunch when the SSM saturates. It was found that the on-axis longitudinal wakefield evolution is highly stable to aspect ratio for both focused and astigmatic bunches, which is promising for error tolerances of those parameters of proton bunches used for electron acceleration. Further numerical and analytical investigation of the coupling between the asymmetry and radial modulation, including for longer bunches with non-uniform longitudinal profiles is ongoing.

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