PIC simulations of high-power THz radiation produced by the collision of profiled plasma wakefields

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Abstract. A PIC model allowing to study generation of THz radiation by the collision of plasma wakes with mismatching small-scale transverse modulation of electrostatic potential are presented in the paper. We discuss the scheme in which each of the profiled wakes is excited by a pair of interfering femtosecond laser pulses copropagating at a small angle to each other. The interference of laser fields produces transverse modulation of the ponderomotive force on plasma electrons resulting in production of wakefields with the small-scale nonuniform structure. In this paper, we generalize the model of virtual laser pulses allowing not to resolve the laser wavelength in order to take into account the effects of laser interference and then implement this model in a 2D3V PIC code in slab geometry. By modeling the collision of plasma wakes slightly shifted in the transverse direction, we show that the power of the produced THz radiation increases with the growth of the laser spot-size, which makes the scheme applicable to most powerful and energetic laser systems and opens the way to generation of gigawatt-level THz pulses.

1. Introduction

The generation of powerful pulses of coherent terahertz radiation is currently relevant both for the study of new fundamental physics associated with the excitation of various collective degrees of freedom in a solid (spin waves, crystal lattice vibrations, photoinduced superconductivity), and for various applications in chemistry, biology, medicine and the security sector. Despite the high demand for sources of such radiation, there is a problem of achieving high values of its power (about 1 GW) and total energy in a pulse (> 1 mJ) within the spectral range of 1-10 THz. This frequency range turns out to be equally inconvenient both for the known vacuum devices and for the methods of quantum electronics. Recently, both the accelerator and laser communities have been actively proposing their solutions for filling the so-called THz gap.

In this paper, using particle-in-cell (PIC) simulations, we study a new scheme for the conversion of high-power laser radiation into low-frequency radiation of the THz range. The scheme is based on the original idea of a head-on collision of two laser-induced plasma wakes proposed in [1]. The essence of the idea is that the nonlinear interaction of two potential plasma waves excited in a homogeneous plasma by counterpropagating laser pulses leads to the emission of electromagnetic radiation at the doubled plasma frequency $2\omega_p$ across the optical axis if the
plasma wakes have different profiles of electrostatic potential. Experimental implementation of the scheme of collision of two short (40 fs) laser pulses with a wavelength of 830 nm and a total energy of up to 0.2 J in a supersonic helium jet has already started at the Institute of Laser Physics SB RAS [2, 3]. However, in a setting that involves the use of axially-symmetric Gaussian beams, this experiment is not scalable to laser systems with much higher pulse energies. The point is that the efficiency of the second harmonic radiation reaches a maximum when the size of the inhomogeneity of the laser radiation intensity in the focal spot is comparable to the plasma skin-length $c/\omega_p$. Keeping the Gaussian profile of laser beams and increasing their energy, we will have to increase their intensity at the focus, which will inevitably lead to the buildup of highly nonlinear wakes with a short lifetime. To obtain radiation with a narrow spectral line, it is necessary to limit the laser fields at the focus to relatively low values of the dimensionless vector potential ($a_0 = 0.7 – 0.8$). Thus, the efficiency and duration of THz generation for laser systems with much higher pulse energy can be preserved either by creating flat laser drivers, for which a narrow intensity profile is retained in one of the directions, or by profiling of large-diameter laser beams at the scale $c/\omega_p$. In this paper, we will perform a PIC simulation of a scheme in which small-scale modulation of the amplitude of each of the colliding wakes is created due to the interference of fields from two co-directional laser pulses propagating at a small angle to each other. To verify the possibility of efficient generation of THz radiation of a gigawatt power level on laser systems of the multi-terawatt and petawatt class, let us investigate whether it is possible to increase the THz radiation power by increasing the transverse size of colliding wakes with a small-scale inhomogeneous structure.

2. Model of virtual laser pulses

For a full-scale simulation of the proposed THz generation scheme, the size of the spatial region in which the nonlinear interaction of counterpropagating wakefields occurs should significantly exceed their wavelength. PIC simulations of the self-consistent evolution of real laser fields with a resolution of the laser wavelength at such macroscopic spatial scales require enormous computational resources; therefore, it becomes necessary to use a simplified approach that takes into account only the slow dynamics of plasma electrons under the action of the ponderomotive force from the laser pulse (model of virtual laser pulses). In a model with the standard PIC algorithms, this approach is implemented via the addition of the ponderomotive force to the equation of motion of plasma electrons under the action of the ponderomotive force from the laser pulse (model of virtual laser pulses). In this model, a pair of co-directional laser pulses propagating at a small angle to each other. To verify the possibility of efficient generation of THz radiation of a gigawatt power level on laser systems of the multi-terawatt and petawatt class, let us investigate whether it is possible to increase the THz radiation power by increasing the transverse size of colliding wakes with a small-scale inhomogeneous structure.

Let a pair of accompanying y-polarized laser pulses propagate in the plasma at angles $\alpha$ and $-\alpha$ to the z-axis with a central frequency $\omega_0$ and envelopes

$$a_s(x, z, t) = a_0 \sqrt{\frac{\sigma_0}{\sigma_s(z_s)}} \exp \left(-\frac{x^2}{\sigma_s(z_s)}\right) \sin^2 \left(\frac{\pi(t-t_0-z_s)}{2\tau}\right) \times \left[\mathcal{H}(t-t_0-z_s) - \mathcal{H}(t-t_0-z_s-2\tau)\right],$$

where $a_0$ is the amplitude of the dimensionless vector potential at the focus of each of the pulses numbered $s$, $\sigma_0$ is the size of their focal spot, $\tau$ is their duration, $\mathcal{H}(t)$ is the Heaviside function, and $t_0 = \sin \alpha \left(L_x - L_z \tan \alpha\right)/2$ is the moment of time when the centers of laser pulses
enter the computational domain with dimensions $L_x \times L_z$ (under zero time we choose the moment when laser wings cross the corners of the computational domain). Due to diffraction, the size of each pulse changes with distance from the focus located in the center of the simulation box ($z = z_0 = L_z/(2 \cos \alpha)$) according to the law $\sigma_s(z_s) = \sigma_0 \sqrt{1 + (z_s - z_0)^2/R}$, where $R = \omega_0 \sigma_0^2/2$ is the Rayleigh length. Coordinate transformations from the systems $(x_s, z_s)$ accompanying laser pulses to the $(x, z)$ system associated with the computational domain are carried out according to the rule

$$
x_s = \left(x - \frac{L_x}{2} + (-1)^{s+1} \frac{L_x}{2} \tan \alpha\right) \cos \alpha + (-1)^s z \sin \alpha,
$$

$$
z_s = (-1)^{s+1} \left(x - \frac{L_x}{2} + (-1)^{s+1} \frac{L_x}{2} \tan \alpha\right) \sin \alpha + z \cos \alpha.
$$

Averaging the equations of motion of plasma electrons over the fast period of laser field variation $(2\pi/\omega_0)$, we find that, on longer time scales (of the order of $\omega_p$), the impact of laser pulses on plasma electrons is reduced to the action of a ponderomotive force, which, in the case of two overlapping pulses, contains not only separate contributions from the high-frequency pressure of each of them, but also a term describing their interference:

$$
F = -\nabla \left[ \frac{a_1^2}{4} + \frac{a_2^2}{4} + \frac{a_1a_2}{2} \cos \left(q(x - L_x/2)\right) \right],
$$

where $q = 2\omega_0 \sin \alpha$ is the wavenumber of transverse modulation of this force. In the linear approximation, this force drives a plasma wake with the electric field

$$
E(r, t) = \int_0^t dt' \sin(t - t') F(r, t').
$$

Since the excited plasma wave is electrostatic $E = -\nabla \Phi$, the potential can be calculated as follows:

$$
\Phi(r, t) = \int_0^t dt' \sin(t - t') \left[ \frac{a_1^2(r, t')}{4} + \frac{a_2^2(r, t')}{4} + \frac{a_1(r, t')a_2(r, t')}{2} \cos \left(q(x - L_x/2)\right) \right].
$$

For the selected laser envelope (1), this integral can be taken analytically. Oscillations of electrostatic potential in the produced wake can be represented as a traveling wave

$$
\Phi(r, t) = \frac{\Phi_0(r)}{2} e^{i(t-z \cos \alpha)} + c.c.
$$

propagating along $z$ with the superluminal phase velocity $v_{ph} = 1/\cos \alpha$ and the amplitude

$$
\Phi_0(r) = -\frac{i e^{-(x + L_x/2 \sin \alpha)^2/4 \sigma_0^2}}{4 [r/\pi + (x/L_x/2)] [r/\pi + (x/L_x/2)]^2} \left\{ 3 \sin \tau \left( e^{-2x^2/\sigma_1^2} e^{-i(x-L_x/2) \sin \alpha} + e^{-2x^2/\sigma_2^2} e^{-i(x-L_x/2) \sin \alpha} \right) \right.
$$

$$
+ \exp\left\{ -\frac{x^2/\sigma_1^2 - x^2/\sigma_2^2}{\sqrt{\sigma_1^2 \sigma_2^2}} \right\} \cos \left(q \left( x - \frac{L_x}{2} \right) \right) \left[ -4 - \frac{x^2}{\pi^2} + \left( 2 + \frac{x^2}{\pi^2} \right) \cos \mu \right] \sin \nu + 3 \pi \sin \mu \sin \nu \right\},
$$

where

$$
\mu = \frac{2\pi}{\tau} \left( x - \frac{L_x}{2} \right) \sin \alpha, \quad \nu = \left( x - \frac{L_x}{2} \right) \sin \alpha - \tau.
$$
Table 1. Performance of calculations.

| Type         | NKS-1P  | NKS-1P  | NKS-1P  | Matrosov | NSU     |
|--------------|---------|---------|---------|----------|---------|
| 2 x Intel Xeon E5-2697A v4 (2.6 GHz, 16 cores), AVX2 | 1331.2 Gflops/s | 3456 Gflops/s | 4454.4 Gflops/s | 1382.4 Gflops/s | 6400 Gflops/s |
| NKS-1P 2 x Intel Xeon Phi 7290 Platinum (2.9 GHz, 24 cores), AVX-512 | 220 Gflops/s | 204 Gflops/s | 680 Gflops/s | 196 Gflops/s | 773 Gflops/s |
| Matrosov NSU 4 x Intel Xeon Gold (2.4 GHz, 20 cores), AVX-512 | 16.5 % to peak | 5.9 % to peak | 15.3 % to peak | 14.2 % to peak | 12 % to peak |

3. PIC model

To simulate the problem, we developed a 2D3V PIC code with open boundary conditions. The movement of particles is carried out according to Boris’s scheme [4] with the addition of a ponderomotive force to the Lorentz force that is created by self-consistent electromagnetic fields. In the case of two accompanying laser pulses with overlapping fields, the ponderomotive force is calculated according to the formula (4). For computational particles, we use the second order form-factor. Electromagnetic fields are calculated on the grid using the FDTD scheme [5]. To absorb electromagnetic radiation, an absorbing layer PML is used [6]. In front of this layer we measure the power of the outgoing radiation by calculating the Poynting vector.

The model of virtual laser pulses allows one not to resolve the laser wavelength. The smallest spatial scale in the considered problem is the plasma skin-length \( c/\omega_p \) which is well resolved with the grid \( h_x = h_z = 0.1 c/\omega_p \). The time-step is \( dt = 0.05/\omega_p \). The appropriate noise level is achieved using 100 computational particles per cell.

Since the total number of particles in the simulation reaches \( 10^9 \), the calculations are carried out using supercomputers NKS-1P [7], Matrosov [8] and NSU [9]. In our code, we have implemented a parallel algorithm using MPI communications and computational load balancing. The main part of the calculations falls on the calculation of particle motion (interpolation of electromagnetic fields to the position of the particle, calculation of the ponderomotive force, determination of the current density during motion), therefore, balancing is performed by redistributing particles and processors with a uniform grid decomposition. PIC codes are memory-bounded, so in addition to the performance of a particular processor, memory access and communication between computational nodes is an important element. We have tested the performance of the used supercomputers on our code.

The Table 1 shows the peak performance of the nodes and the estimated performance of our code. As one can see from the table, the new processors supporting the avx-512 can achieve comparable results in terms of efficiency. The exception is Intel Xeon with low frequency.

4. Simulation results

First, let us study how accurately the wake amplitude (8) predicted by the linear theory is reproduced in our 2D3V PIC model. In these simulations, we inject two copropagating laser pulses with the following fixed parameters \( a_0 = 0.5, \omega_0 = 25.44, \tau = 3.48 \) into a uniform density
plasma that initially has the Maxwellian distribution of electrons with the temperature 14 eV and locates in the center of the simulation box \( L_x \times L_z = 160c/\omega_p \times 400c/\omega_p \). In relation to typical parameters of the experiments in ILP SB RAS, the choice of the dimensional laser frequency corresponds to the certain plasma density \( 2.5 \cdot 10^{18} \text{ cm}^{-3} \). Figure 1 shows the spatial structure of plasma wakes excited by laser pulses with different spot-sizes \( \sigma_0 \). The transverse profile of wake amplitude realized in PIC simulations is seen to agree well with the theoretical prediction.

For efficient generation of \( 2\omega_p \)-radiation, plasma wakes propagating in opposite directions should have differing profiles of potential \( \Phi_1(\mathbf{r}) \neq \Phi_2(\mathbf{r}) \), since a radiating nonlinear current is determined by

\[
J_\parallel \propto \Phi_1 \Delta_{\perp} \Phi_2 - \Phi_2 \Delta_{\perp} \Phi_1.
\]  

A simple way to realize differing amplitude profiles in such a scheme is to shift one wake relative to the other along the \( x \)-direction. In other words, wakes should collide with some impact parameter. The optimal value of such a shift for the collision of wakes produced by single laser pulses [1] is found to be comparable with the inhomogeneity scale of wake amplitude. Theoretical solution of the same problem for the profiled wakes will be the subject of our future work. Figure 2 (a), (b) and (e), (f), (f) does really confirm that collision of wakes without transverse shifting for \( \sigma_0 = 10 \) turns out to be much less efficient for electromagnetic emission than the case of the finite shift \( \Delta x = \pi/(2\sqrt{3}) \) indicated in Figure 2(i). Since our goal is to produce radiation effectively in plasma volumes as large as possible (at least, much greater in sizes than \( c/\omega_p \)), it is naturally to assume that the maximum work performed by the modulated nonlinear current over the field of radiated electromagnetic wave should be achieved when the period of current modulation equals to the radiation wavelength. Since the wavenumber of electromagnetic wave at the second harmonic of the plasma frequency equals to \( \sqrt{(\omega/\omega_p)^2 - 1} = \sqrt{3} \), this resonance condition has the form \( q = \sqrt{3} \). To get in such a resonance, the angle between pulses should equal to \( \alpha = \arcsin(\sqrt{3}/(2\omega_0)) \).

Figure 1. Excitation of profiled wakes by laser pulses with different spot-sizes \( \sigma_0 \). (a) Maps of the longitudinal electric field \( E_z(x, z) \) in the moment of time \( t = 196/\omega_p \), (b) transverse profiles of wakefields \( E_z(x) \) at \( z = 187.5c/\omega_p \) in PIC simulations and in the linear theory (5).
Figure 2. Generation of $2\omega_p$-radiation by profiled plasma wakes. Top row: maps of electric field $E_z(x, z)$ for different $\sigma_0$. Middle row: maps of magnetic field $B_y(x, z)$ for different $\sigma_0$. Bottom row: overlapping of colliding wakefields for the shifted wakes with $\sigma_0 = 10$ at the focus $z = 200 c/\omega_p$, electric field $E_z$ of radiation wave measured in a single point as a function of time in all cases, Fourier-spectra of these fields, total radiation power escaping from the simulation box as a function of time in all cases.

Simulations with greater spot-sizes (see maps of EM fields in Fig. 2(c), (d), (g), (h)) demonstrate the increase in the total radiation power $P$ (Fig. 2(l)) generated in the whole computational domain with the growth of laser beam size. This effect is seen to be associated not only with higher radiation fields (Fig. 2(j)), but also with a longer duration of emission. The produced radiation has a narrow spectral line and is really concentrated near $2\omega_p$ (Fig. 2(k)).

To calculate the efficiency of laser-to-THz energy conversion ($\eta = E_{THz}/E_L$), one should divide the total energy radiated at $2\omega_p$ ($E_{THz} = \int Pdt$) by the energy contained in four laser beams

$$E_L = \frac{3}{2} \sqrt{\frac{\pi}{2}} a_0^2 \omega_0^2 r \sigma_0.$$

Figure 3 shows some decrease in efficiency with the growth of laser spot-size $\sigma_0$, but the absolute value of this efficiency turns out to be tens times higher than in the original scheme without profiling. It needs more research to verify if the decrease in efficiency is not an effect of the limited length of our computational domain.

5. Conclusion

It is shown that the power of THz radiation in the scheme of colliding plasma wakes can be increased with the increase of energy and spot-size of laser drivers if electrostatic potential in these wakes is profiled with the typical scale $c/\omega_p$ and these profiles are considerably shifted relative to each other across the propagation axis. More research needed to find the optimal impact parameter of wakes collision and optimal laser intensities, but, based on the first
Figure 3. Laser-to-THz energy conversion efficiency as a function of time for different $\sigma_0$.

simulations, we can already conclude that the proposed method of wake profiling makes the THz generation scheme scalable to high-energy laser systems.

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