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METHODS FOR NUMERICAL NOISE MITIGATION IN QUASISTATIC THREE-DIMENSIONAL PARTICLE-IN-CELL CODE LCODE3D

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Abstract

We discuss a new quasistatic 3D particle-in-cell code LCODE3D for simulating plasma wakefield acceleration, which is a modified version of the quasistatic 2D3V code LCODE, focus on the numerical noise of the plasma solver and propose methods for reducing it. We compare different particle shape functions, as these functions affect the code stability. We also introduce the so-called dual plasma approach, which improves stability and dampens small-scale noise. After applying the proposed methods, the results of the new code closely agree with LCODE simulation results.

INTRODUCTION

Plasma wakefield acceleration with a particle driver (PWFA) is an actively developing method of accelerating charged particles over short distances [1, 2]. Experience from numerous studies has shown that the quality design of new experimental PWFA facilities demands numerical calculations. Simulation codes provide extensive opportunities for studying plasma dynamics under conditions close to experimental. However, while many codes can simulate experiments that require a short computational window, there is a shortage of reliable codes that are capable of simulating long-term wakefield evolution. These codes should provide low numerical noise with a reasonable consumption of computer resources, which presents significant challenges in code development.

One of the already benchmarked codes for simulating a long-term wakefield evolution [3, 4] is LCODE [5, 6]. The bedrock of LCODE computational algorithm is the particle-in-cell method (PIC) and the quasistatic approximation [7]. The latter significantly reduces the simulation time. However, LCODE allows only two-dimensional simulations in Cartesian or axisymmetric geometry. Therefore, we are developing a modified version of LCODE — LCODE3D, which has the following main features:

- 3D Cartesian geometry,
- co-moving simulation window that moves with the light velocity c,
- field-based kinetic plasma solver,
- quasistatic approximation.

The quasistatic approximation takes advantage of the fact that the plasma evolves much faster than the beam in the cases of interest. Therefore, we separate the calculation of plasma response and beam evolution. However, when calculating the plasma response, we encounter numerical noise that is related to the motion of plasma electrons. In long simulation windows, the noise begins to dominate the physical processes, and simulation results become unreliable. The noise in PIC codes may be of a different nature, related to the numerical solution of Maxwell's equations [8], the plasma "self-heating" [9], or something else. At the moment, none of the developed methods can completely suppress the noise. Different methods are needed to deal with different types of noise.

WAYS TO REDUCE THE NOISE

A Dual Plasma Approach

One of the numerical effects leading to a noise increase is merging of plasma macro-particles. The merging occurs in an initially cold plasma, because the interaction between particles is calculated incorrectly if they are in the same cell.

We propose a new method of dealing with this problem: the dual plasma approach, which is essentially a description of plasma components in Lagrangian coordinates. The idea is to represent the plasma in simulations with two sets of particles (Fig. 1). The first set consists of sparsely spaced "real" particles, for example, one particle per 4 or 9 cells. These particles advance as normal particles in the PIC method. The second set is "virtual", with many particles per cell, and exists only at the stage of calculating plasma charge and currents. The parameters of these particles are obtained from the first set by bilinear interpolation of parameters of neighboring "real" particles. Near the free plasma boundary, the parameters of "virtual" particles are determined by one or two nearest "real" particles.

Smoother Shape Function

Typically, PIC codes use the parabolic shape function for plasma macroparticles. However, in quasistatic simulations of the long-term wakefield evolution, plasma particles cross the boundaries between cells many times. Each transition results in a numerical error, which occurs because the shape function is not infinitely differentiable, and accumulates with time. To reduce the error, we suggest using a higher-order shape function for both charge and current deposition and field interpolation. The following shape function has a third

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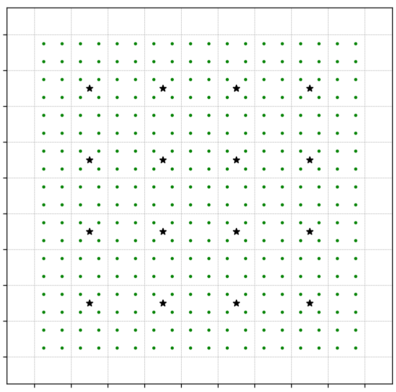
order of continuity and generates less noise:

$$R(x) = \begin{cases} \frac{1}{24}\left(\frac{x}{h}+\frac{5}{2}\right)^4, & -\frac{5}{2} \le \frac{x}{h} < -\frac{3}{2}, \\ \frac{55}{96} - \frac{5x}{24h} - \frac{5x^2}{4h^2} - \frac{5x^3}{6h^3} - \frac{x^4}{6h^4}, & -\frac{3}{2} \le \frac{x}{h} < -\frac{1}{2}, \\ \frac{115}{192} - \frac{5x^2}{8h^2} + \frac{x^4}{4h^4}, & -\frac{1}{2} \le \frac{x}{h} < \frac{1}{2}, \\ \frac{55}{96} + \frac{5x}{24h} - \frac{5x^2}{4h^2} + \frac{5x^3}{6h^3} - \frac{x^4}{6h^4}, & \frac{1}{2} \le \frac{x}{h} < \frac{3}{2}, \\ \frac{1}{24}\left(\frac{x}{h}-\frac{5}{2}\right)^4, & \frac{3}{2} \le \frac{x}{h} < \frac{5}{2}, \\ 0, & |x| > \frac{5}{2}h, \end{cases} \tag{1}$$

where h is the grid step size.



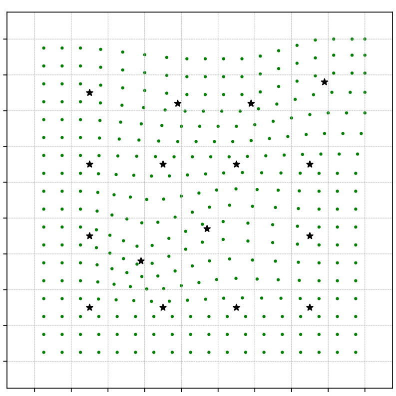


Figure 1: Schematic arrangement of "real" (black stars) and "virtual" (green dots) macro-particles using the dual plasma approach.

BENCHMARKING

To check the correctness of the plasma solver calculations, we use the so-called AWAKE Test 1 [10]. The test examines the long-term evolution of a low-amplitude plasma wave generated by a short proton beam. The beam shape does not change in the co-moving simulation window and is defined analytically:

$$n_b = \begin{cases} \frac{n_{b0}}{2} e^{\frac{-r^2}{2\sigma_r^2}} \left[1 - \cos\left(\sqrt{\frac{\pi}{2}}\frac{\xi}{\sigma_z}\right)\right], & -\sqrt{2\pi} < \frac{\xi}{2\sigma_z} < 0, \\ 0, & \text{otherwise}, \end{cases} \tag{2}$$

where we use the Cartesian coordinates (x, y, ξ) with the co-moving coordinate $\xi = z - ct$ instead of the direction of beam propagation z. The beam parameters are

$$\sigma_r = c/\omega_p, \quad \sigma_z = c/\omega_p, \quad n_{b0} = 0.1n, \tag{3}$$

where $\omega_p = \sqrt{4\pi n e^2/m_e}$ is the plasma frequency, n is the plasma density, m_e is the electron mass, and e is the elementary charge. Plasma ions are immobile.

We make simulations with the "conventional" PIC solver with parabolic-shaped particles and the "improved" solver that incorporates the dual plasma approach and higher-order shape function. In both cases, the window width is $15.37c/\omega_p$ in transverse directions, the grid steps are $dx = dy = d\xi = 0.01c/\omega_p$, and 90 601 "real" macro-particles for plasma electrons are used.

We focus on two parameters: wave amplitude, which must be nearly constant over hundreds of wave periods (Fig. 2), and wave period, which must be close to $2\pi\omega_p^{-1}$. The wave amplitude can be approximately calculated with the linear wakefield theory [11], but here we aim for greater accuracy and compare our results with high-resolution LCODE simulations (with the grid steps $dr = d\xi = 0.005c/\omega_p$), which accounts for nonlinear effects.

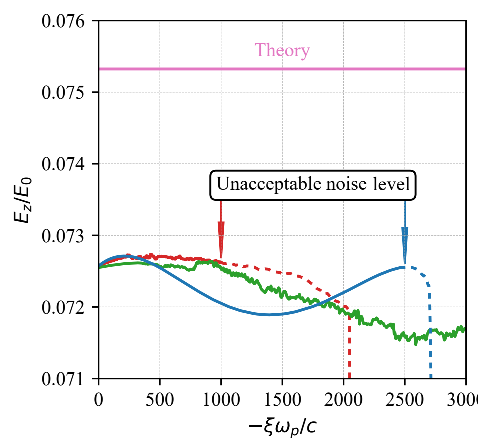


Figure 2: Positive local extrema of the on-axis electric field E_z in test 1 calculated with LCODE (green line), LCODE3D with conventional (red line) and improved (blue line) solvers.

According to the linear theory, the longitudinal electric field on the axis oscillates with the constant amplitude $E_{z,max} = 0.07532E_0$, where $E_0 = m_e c\omega_p/e$. Because of nonlinear effects, the amplitude in simulations is lower. Both conventional and improved solvers reproduce this amplitude reduction at the same accuracy as LCODE. The wave period also depends on nonlinear effects [12] and in both cases is longer than $2\pi\omega_p^{-1}$ by 0.07%, which is close to the value of 0.053% obtained with LCODE. The difference probably arises from the different geometry of the codes or different resolution. The two-dimensional maps of the field E_z after a long time of wave evolution also show good agreement between the codes, if we correct for the small difference in periods (Fig. 3).

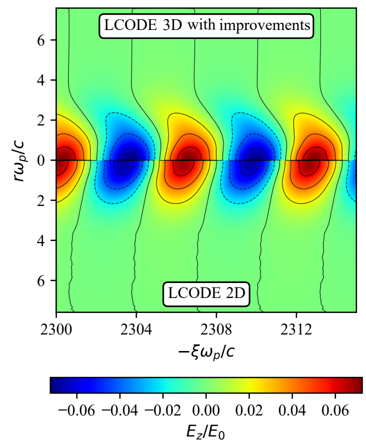


Figure 3: Comparison of field profiles after a long-term wave evolution.

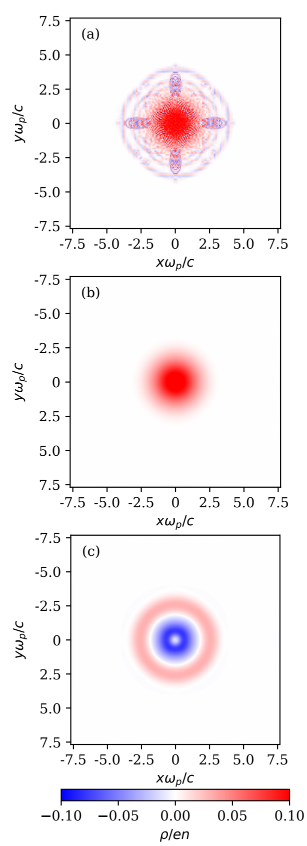


Figure 4: Transverse distributions of the plasma charge density: (a) the conventional solver, $\xi = -1000c/\omega_p$, (b) the improved solver, $\xi = -1000c/\omega_p$, and (c) the improved solver, $\xi = -2300c/\omega_p$.

The difference between the conventional and improved solvers is seen in transverse distributions of the plasma charge density (Fig. 4). The conventional solver produces a highly noisy result, and this noise eventually leads to a rapid wave destruction (Fig. 2). The improved solver is also not free from the noise, and this noise also leads to the wave destruction. However, the wave amplitude and plasma density profiles are reproduced correctly almost until the wave collapses.

To conclude, with the discussed noise reduction methods, it is possible to simulate the wakefield evolution with the quasi-static three-dimensional code LCODE3D for as long as several hundred wave periods.

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