Initialization of charged particle beam in OSIRIS

A. Balzarini[1,2], R.A. Fonseca[2,3], J. Vieira[2], E. Boella[2], L.O. Silva[2]

[1] *Dipartimento Energia, Politecnico di Torino, Turin, Italy*

[2] *GoLP/Instituto de Plasmas e Fusão Nuclear - Laboratório Associado, Instituto Superior Técnico, Lisboa, Portugal*

[3] *ISCTE - Instituto Universitário de Lisboa, Lisboa, Portugal*

Introduction

There are several phenomena that can be investigated looking at the interaction between a particle beam and a plasma. One important example is that of beam plasma accelerators, where a particle beam acts as a driver for wakefield acceleration in the plasma. The tools of choice for modeling these scenarios are particle-in-cell (PIC) codes such as OSIRIS[1], that is a fully relativistic, massively parallel, PIC code. The current algorithm for initializing the EM fields associated with the beam implemented in OSIRIS works by gradually accelerating the beam, and has some limitations, in particular regarding the computational time required to converge to a solution. In this work we present a new algorithm that overcomes this problem, leading to an improvement of the code performance and of the accuracy of the initial fields.

Initialization of EM-fields in PIC code

Electromagnetic PIC codes generally work by iteratively advancing particles and fields in time starting from a self-consistent description of the system. The default is to initialize it assuming that it is charge and current neutral, with no EM fields present. This is not suitable for simulating a charged particle beam, where beam current and charge are expected to generate both electric and magnetic fields. To initialize the values of fields associated with the beam, the current algorithm in OSIRIS would accelerate the beam, from zero to the velocity correspondent to the required Lorentz factor γ, through a finite number of time-steps[1]. During this initialization stage, the beam would not react to simulation fields, that would gradually converge to a value close to the real one, especially for large number of initialization time-steps. Although this scheme was easy to implement, it had some problems: the algorithm converges very slowly, so the initialization stage requires significant time that is not negligible when compared with the total simulation time. The number iterations required also grows on the size of the simulation box, further slowing larger simulations.

[1]This mimics the gradual acceleration of a beam in a constant field.

New algorithm

The goal of the new scheme is to evaluate, at time $t = 0$, the EM field associated with a particle beam that is moving in x_1 direction with an high γ. Following the existing OSIRIS code, the new algorithm is parallelized[2] and it is written for 2D-cartesian, 3D-cartesian and 2D-cylindrical coordinates (axial-symmetrical). The steps that the new algorithm does are:

1. The charge density, the velocity of the beam and the geometrical parameters of the system are moved from the laboratory reference frame, where the beam has its γ, to the beam reference frame, where its velocity is 0, using the Lorentz transformation. With the hypothesis that the particles are moving in x_1 direction, the result of the transformation is only a stretch of the space along x_1 by a factor γ and a consequent reduction of the charge density, ρ.

$$x_1' = \gamma x_1; \quad x_2' = x_2; \quad x_3' = x_3; \quad \rho' = \frac{\rho}{\gamma}; \tag{1}$$

Since we are dealing with beams that are ultra relativistic, with $\gamma \gg 1$, the cell shape in the beam reference frame will be significantly stretched along the x_1 direction leading to $dx_1' \gg dx_2' \simeq dx_3'$. As result, we can consider a cell in this frame like an infinite rod along the x_1 direction.

2. On the beam reference frame the velocity is zero, making this an electrostatic problem. Therefore it is possible to evaluate the electric field, **E**, using Gauss's law, that, expressed in OSIRIS normalized units, is:

$$\int \mathbf{E} \cdot \mathbf{dS} = \int \rho dV \tag{2}$$

Considering that each cell is an infinite rod we get for a 2D-cartesian case:

$$E_2 = \frac{\rho' \cdot dx_2'}{2} \tag{3}$$

And for 2D-cylindrical/3D-cartesian one:

$$E(r) = \frac{\rho' \cdot dx_2' \cdot dx_3'}{2 \cdot \pi \cdot r} \tag{4}$$

Due to the stretching of the grid, two grid-points that lie in x_1 direction are too far to influence each other. As consequence the E-field is only evaluated in a plane perpendicular to x_1, the direction of the motion of the charge, while is set to zero elsewhere. Then, since each charged cell is approximated to an infinite rod, there is no E_1 component of the field, and it is set to zero everywhere. All this cumulative effects lead to a speed-up of the code.

3. Once all the components of the electric field are evaluated, it is possible to come back to the laboratory frame of reference using again the Lorentz transformation applied to the fields:

$$\mathbf{E}_\perp = \gamma \cdot \mathbf{E}'_\perp; \quad \mathbf{B}_\perp = \frac{\mathbf{v}}{c} \times \mathbf{E}; \tag{5}$$

[2]For distributed memory systems, using MPI.

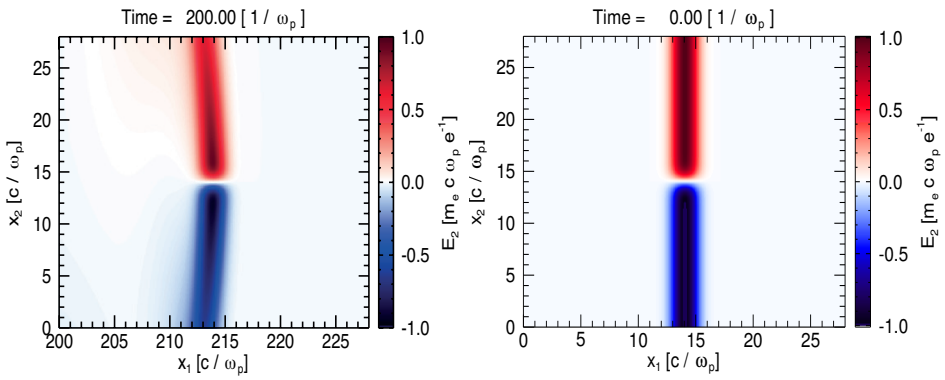

Figure 1: E_2 of a 2D gaussian positron beam propagating in x_1 direction obtained with the traditional algorithm (left) and the new one (right). 512×512 cells, 2×2 particles per cell, 4 nodes. The time required to obtain the result on the left is 165 s, 10000 time-steps, while for the other one is less than 0,1 s.

Giving the staggering of field values in the Yee mesh used by OSIRIS, we need to center some of them, which we do by linear interpolation. A comparison between the new algorithm presented here and the traditional one for a 2D case, can be seen in fig. 1.

Parallelization

OSIRIS was designed from scratch to be massively parallel, so it could tackle large simulation problems. The traditional algorithm required no additional effort to parallelize, as it only involved the accelerating local particles. In the new algorithm however, careful attention needs to be given to this issue, as the charge of the beam in one particular parallel node may influence the fields in other ones. One possible approach would be broadcast the charge from a given nodes to all the nodes and then calculate the corresponding fields locally, repeating for all source nodes. However, given that the field lines lie in planes perpendicular to the direction x_1, so they have the same x_1 coordinate of the charges that contribute to their generation, this would be inefficient, as most of the nodes would not be doing any work.

Considering our specific problem it is possible to improve the parallelization efficiency by dividing the domain using the MPI communicators, so that these will have inside only the nodes characterized by the same x_1 coordinate. In this way the information about the charge inside a communicator is only broadcast to nodes that are all also inside, but not to all the others. As result we have a significant speedup of the code, leading to an almost linear performance increase with the number of nodes in x_1 direction.

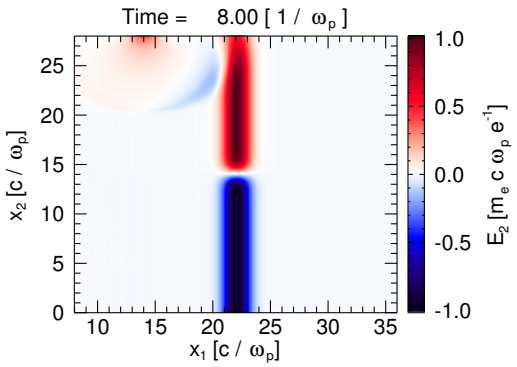

Figure 2: E_2 component of a 2D gaussian positron beam propagating in x_1 direction, it is possible to see the difference between the upper boundary (without PML initialization) and the lower one (with PML initialization).

Absorbing boundary conditions

Beam plasma simulations are generally performed using some form of absorbing boundary conditions for the fields, to simulate open space boundaries. In OSIRIS perfectly matched layer (PML) absorbing boundary conditions[2] are used, implementing in particular the version described here [3]. Inside the PML, we use a modified version of Maxwell's equation that define a medium with vacuum impedance but with gradual damping, so that EM waves leave the simulation box and are damped without being reflected. To avoid spurious reflection in these boundaries, we also need to initialize the beam field values inside the PML, matching not only the particle beam conditions, but also the specific medium properties in this region. Fig. 2 illustrates the effect of this initialization.

Conclusion

We developed a new algorithm in OSIRIS allowing for the initialization of the EM-fields associated to a highly relativistic charged particle beam. The new scheme is parallelized and can work with PML boundary conditions. The main advantage of the new scheme is an improvement in the speed of the code that can be, depending on the problem, up to three order of magnitude faster. Moreover, while the previous algorithm gives only an approximation of the EM-field values, the new algorithm evaluates their exact values at time zero.

References

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