OPTIMISATION OF PARTICLE-IN-CELL SIMULATIONS FOR LASER WAKEFIELD ACCELERATION

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The aim of this study is to find out the most suitable parameters for improving the accuracy of a Particle-in-cell (PIC) simulations for laser wakefield acceleration in gaseous target. We refer mainly to the grid parameters, the number of cells on horizontal and vertical grid, but also to the number of particles per cell. Our results show that for the same simulation but for different number of cells on the grids, the values of the electron output energy differes and approaches different convergence zones. Besides, we investigated the change of the simulation duration as a function of the number of MPI processes, in order to find the most efficent number in the case of our machine.

Keywords: laser wakefield acceleration, electron energy, grid, PIC

1. Introduction

The study of laser wakefield acceleration has constantly grown in interest after its discovery by Tajima and Dawson 1979 [1] and along with the creation of more powerfull laser of PW-order (Papadopoulos et al. 2019)[2] and a state-of-the-art 10 PW peak power femtosecond laser pulses at ELI-NP nowadays (Radier et al. 2022)[3]. Its potential of accelerating particles up to GeV-energies cm-order distances, compared to tens of meters in an ordinary radio-frequency accelerateor, make this tehnique a highly inovative one with significant potential for the future research (Tanaka et al. 2020)[4].

The principle of the technique is that a high power laser with a non-linear varying electric field profile entering an underdense plasma - i.e. a plasma with the oscillation period longer than the one of the elecrtomagnetic wave entering it - will expell the electrons to the back of the pulse because of the action of the ponderomotive force. This force is generated by the oscillation of the electric field of the laser and because the oscillation is non-linear, on one half of the oscillation where the field is stronger, the electrons experiences a stronger force while in the other half of the oscillation where the field is weaker the force can not completely compensate the effects of the stronger force. Thus, it makes the electrons move to the areas where the field is weaker and not oscillate around a point as in the case of linear harmonic oscillations. The ponderomotive force acts in the same way on the ions but because they are much more heavier than electrons we consider them practically immobile. Thus, the electrons expelled to the back of the pulse creat an ions cavity or a bubble and because of the potential difference created by their separation from the ions, they can be highly accelerated if injected or self-injected into this bubble. This structure travels along with the pulse and the electrons may be accelerated to energies of order of 1 GeV over distances of cm-long order (Leemans et al. 2006)[5].

The most efficient tool used to deal for the descprition of such systems large number of particles is the particle-in-cell method. Their main idea is that collections of particles are replaced by a smaller number of pseudoparticles, thus simplfying the computations. The electromagnetic

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fields generated by the motion of such pseudoparticles are derived via the finite-difference time-domain method (or Yee's method) using a staggered grid, and the resulted forces are utilezed to update the velocities and the positions of the pseudoparticles.

In this paper we aim to investigate the optimisation of the PIC simulations for laser wake-field acceleration of electrons in the code EPOCH , described in Arber et al. 2015 [6], and better understand how the change of the grid parameters and number of particles per cell, influence the results and the accuracy of the simulations. Along with these we also analyse how the change in the number of MPI (Message Passing Interface) processes on the simulation machine determines a shorter or longer time of simulation.

2. **Simulation and results**

Our simulations were performed in EPOCH code (Bennett et al. 2017)[7] on the servers of Politehnica University of Bucharest. We investigated the variation of the electron output energy in dependence with the variation of number of cell on horizontal and vertical axis, as well as the number of particles per cell. The Gaussian laser used in simulations is characterized by the wavelength $\lambda_0 = 0.8\,\mu\text{m}$, the spot diameter $D_0 = 25\,\mu\text{m}$, the intensity $I = 4 \times 10^{20}\,\text{W/cm}^2$ and the pulse duration $\tau = 25\,\text{fs}$. The dimensions of the moving simulation window are $\Delta X = 230\lambda_0$ and $\Delta Y = 78\lambda_0$. The He plasma used has the electron density $n_e = 1 \times 10^{18}\,\text{cm}^{-3}$ and the ion density is $n_i = 0.5 \times 10^{18}\,\text{cm}^{-3}$, while the simulation time is 10 ps in the first set and reaches 14 ps in the last one. We performed severel sets of simulations, in order to see the variations of electron output energy as a function of the varied parameters, at first varying the number of cells on horizontal grid, on vertical one and the number of particles per cell. Then, we selected the appropriate dimensions in order for the cells to be squares and then increase the number of cells keeping them squares. The results give us a guide of optimising the parameters in order the obtain better results in a time as short as possible.

The first set of simulations was performed by varying the number of cells on horizontal grid (nx), taking the values 3300, 3600, 3900 and 4100 while keeping constant the number of cells on vertical grid (ny), and the number of particles per cell: 6 electrons and 3 ions. The obtained results are presented in Figure 1, while in Figures 2 and 3 we show the plots for the energy distribution and number density respectively, for the first case at 10 ps simulation time.

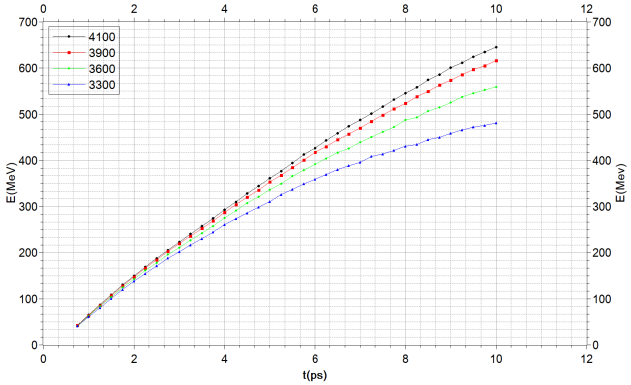

Fig. 1. The variation of the electron energy for different values of the number of cells (nx) on horizontal grid

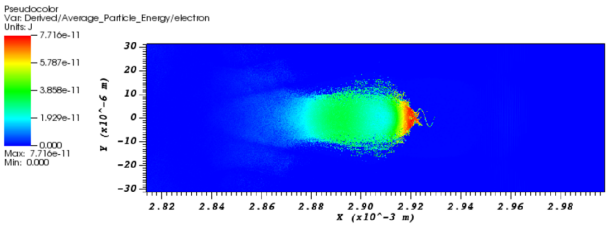

Fig. 2. The energy distribution map for the case with 3300 cell on horizontal grid, after 10 ps

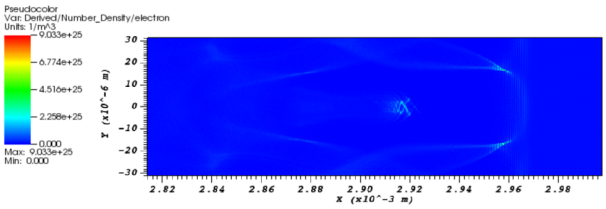

Fig. 3. The corresponding number density map for the above case

Hence, it is observed that by increasing the number of cells in the horizontal axis (the direction of light propagation), the accuracy and thus, the electron output energy obtain increases along with the number of cells. Despite the simulation time increases significantly, the simulation increases its accuracy until approaching a convergence zone, thus the further increase of number of cells ceases to bring significant impovement, while just enlarging the time of performing the simulation.

In the second set of simulations we varied the number of cells on the vertical grid, ny, taking the values 700, 900, 1000, 1100, while keeping constant the number on horiziontal grid at $nx = 3300$. In this case, the number of electrons and ions per cells was kept the same, 6 and 3 resepctively. However, in this case the results presented in Figure 4, show that the energy was decreasing with the increase of the number of cells on vertical direction. Thus, the tendency is of approaching a convergence zone where the values are lower. We present also in Figure 5 and Figure 6 the energy and number density of electrons plots for the last measurement at 10 ps simultaion time.

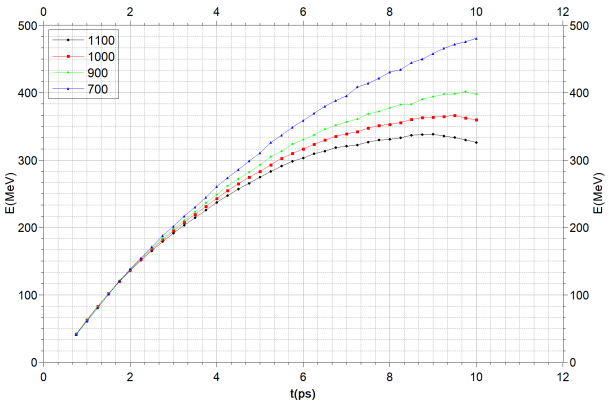

Fig. 4. The variation of the electron energy for different values of the number of cells (ny) on vertical direction

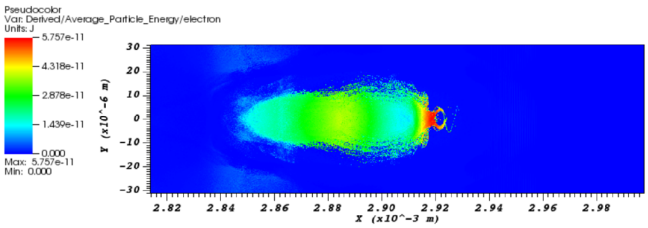

Fig. 5. The energy distribution map for the case with 1100 cell on vertical direction, after 10 ps

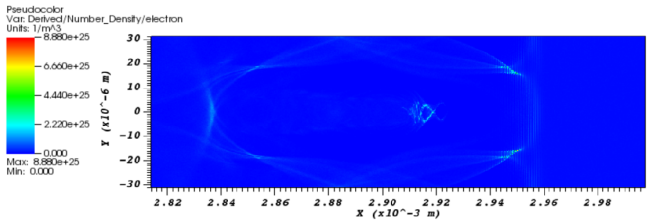

Fig. 6. The number density map in the abose situation

Further, we investigated the differences of the obtained energy when varying the number of electrons and ions per cell. We performed three simulations where the number of electrons and ions per cell where 8 and 4 respectively, 6 and 3 and for the last 4 and 2. In all these three cases we kept constant the number of cells on horziontal grid, $nx = 3300$, and on vertical grid, $ny = 700$. The graphical representation of the results, in Figure 7 show that there is no significant difference between them, thus a further utilization of the lower value of 4 electrons and 2 ions per cell would be more convenient. Besides, we present the plots for the energy and number density for the third case at 10 ps in Figure 8 and 9, respectively.

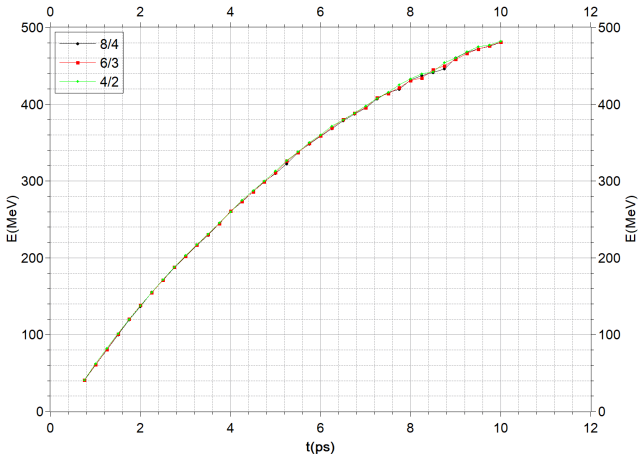

Fig. 7. The variation of the electron energy for different values of the number of electrons and ions in a cell, 4 electrons and 2 ions in the first case, 6 and 3 in the second and 8 and 4 in the last

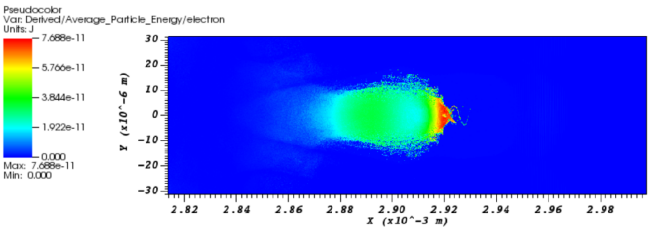

Fig. 8. The energy distribution map for the case with 3300 cell on horizontal direction, 700 on horizontal direction and 8 ions and 4 electrons per cell, after 10 ps

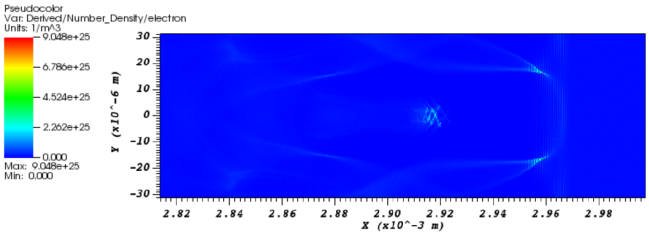

Fig. 9. The number density map for the above case

Following the above obtained results, we pursue to investigate the variation of the energy in the case of the variation of the number of cells on both horizontal and vertical grids. Thus, we considered values of the number of cells such that the cells have a squared form and extract the values of the energy for the five s imulations. Our results are presented in Figure 10, with the plots of energy and number density in Figure 11 and 12, respectively. Thus, we observed a growing of the electron energy with the growth of the number of cells, until reaching a maximum energy zone.

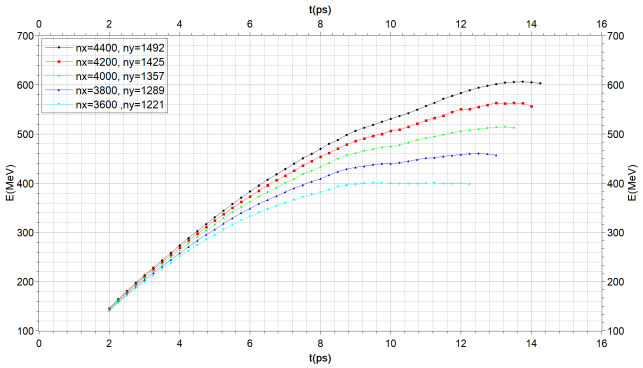

Fig. 10. The variation of the electron energy for different values of the num-ber of cells on both horizontal and vertical grids

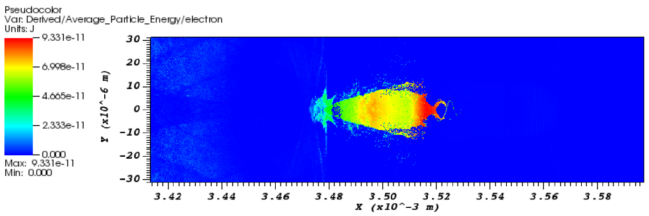

Fig. 11. The energy distribution map for the case with $nx = 4400$ cell on horizontal direction and $ny = 1492$ on vertical direction, after 12 ps

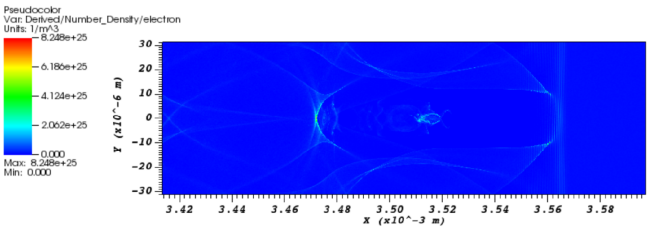

Fig. 12. The corresponding number density of electrons map in this case

Discussion of accuracy

There are several types of inaccuracies in a Particle-in-cell algorithm may appear. One of them are the spatial inaccuracies, determined by the dimensions of the number of cells on the grid, thus on the dimensions of the cells-which, of course, should be as close to reality as possible. The same thing implies for the number of particles per cell. Another possible source of error is the time-step interval, which must satisfy the Courant–Friedrichs–Lewy condition, which in two dimensions writes as:

$$\Delta t \leq \frac{1}{c} \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}},$$

where, $\Delta x = \Delta X / nx$ and $\Delta y = \Delta Y / ny$ and EPOCH gives it by default as 0.95 of the maximum value possible, which was also used by us in these simulations. This condition is necessary in order for every speed in the set-up not to exceed the speed of light. Thus, the smaller the time interval is, the more accurate is the particle pusher algorithm, in this case the Boris push (Boris et al. 1970)[8]. In addition to these, errors may occur because of the algorithm used by code, however, the Boris algorithm despite it is not symplectic, it is volume preserving in the phase-space, which means that the algorithm maintains its accuracy after increasing the number of steps (Qin et al. 2013)[9]. One may also see the comparison made by Ripperda et al. 2018 [10] between different particles pushers, such as Boris, Vay, Higuera-Cary or other integration methods.

An additional condition, besides CFL, that must be fulfilled, was derived by Arefiev et al. 2015[11], and states that the time step

$$\Delta t \ll \frac{\lambda}{a_0 c},$$

where a_0 is the normalized laser amplitude, λ the wavelength of the laser and c the speed of light. In our cases this condition proved to be less restrictive then the CFL condition, even for the lower numbers of cells per grid, 3300 and 700 resepctively. However, this condition, despite not being so restrictive for a large enough number of cells, helps us to better understand why the time step and

the grid step matter for the Boris algorithm. The Boris algorithm splits in two parts the acceleration given by the electric field on the electron and puts in between the rotation given by the magnetic field. If the time step interval of the simulation is not small enough, the angle of rotation in a step will aproach π radians, thus too large too avoid errors. In our simulations, keeping the time step at the given value by default in EPOCH i.e. 0.95 of maximum value allowed by CFL, means that the time step will decease along with the decease of the dimensions of cell, Δx and Δy, respectively. Hence, by enlarging the number of cells per grid, we also enhance the conditions to fulfill the relation derived by Arefiev et al. 2015.

Hence, by having a larger grid step, if the time step is calculated in the same way, it results also in an increase of the time step beyond the threshold of Arefiev et al. 2015, thus, generating larger inaccuracies. The effects on the energy of the laser wakefield accelerated electrons differ when varying the number of cells on the two grids, growing until a convergence zone in the case of horizontal grid and by contrary decreasing until a convergence zone in the case of vertical grid.

2.1. Computational optimisation

In order to optimise the execution time of each simulation, and since EPOCH uses Open Message Passing Interface (OpenMPI) library, we have experimented with custom parameters, $nx = 1500$, $ny = 500$, $t_{end} = 298$ fs for a wide range of numbers of MPI processes. Simulations were performed on the computing cluster of the Polytechnic University, using the haswell-wn32.grid.pub.ro machine, which has 2 sockets, each equipped with an Intel(R) Xeon(R) CPU E5-2640 v3. Our results show in Figure 13 that the optimal configuration for this machine is around 14 MPI processes(with 115.74s duration, as opposed to the serial time of 610.49s), for which the speedup achieved is approximately 5.2.

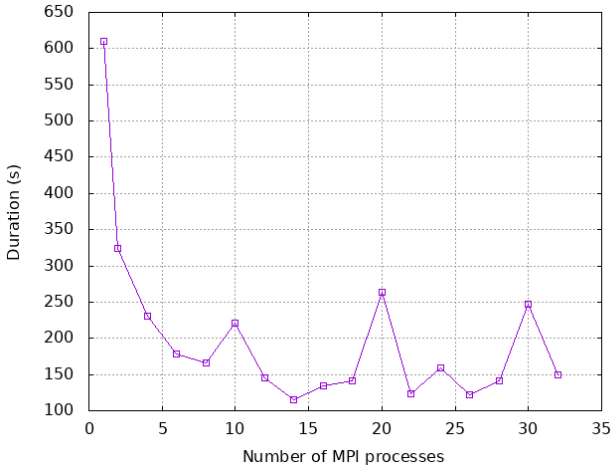

Fig. 13. The time duration of the simulation in dependence with the number of MPI processes

3. Conclusion

Our study has shown that the grid parameters in a PIC simulation play a highly important role in the accuracy of the obtained results. For the case of increasing the number of cells on horizontal grid, the electron energy was increasing tendind to approach a convergence zone. On the other hand, the variation of cells on vertical grid showed an opposit behavior, the energy tendind to approach a convergence zone by decreasing with the increase of the number of cells. The variation of the number of particles per cell, on the other hand, has brought minimum change, thus in further simulations we

can chose to utilize the lower numbers, 4 electrons and 2 ions, in order to decrease the computational power demanded. In our final set of simulations when we increased the number of cells on both grids, in a proportional way, such that the cell remained squared, and we observed that the growth in energy prevails, as in the first case, and it increases until approaching a convergence zone. Not less important when performing simulations, is to find out the most suitable number of MPI processes such that the simulation is the most rapid. For our machine the number turned out to be 14.

Considering the all above results, one my be able to find a balance between the accuracy needed by increasing the number of cells and the computational time to an optimal value.

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