PIC SIMULATIONS OF LASER ION ACCELERATION VIA TNSA

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INTRODUCTION

The acceleration of ions with lasers up to energies of 60 MeV has been successfully demonstrated at different laser systems worldwide, including our facility: PHELIX [1]. The undergoing mechanism is understood as Target Normal Sheath Acceleration (TNSA) [2]. Due to the small transverse emittance and low installation cost laser-ion acceleration is a promising alternative to RF accelerators with the possible application in ion cancer therapy [3]. This contribution is devoted to the numerical investigation of the proton acceleration via the TNSA mechanism using 1D and 2D particle-in-cell electro-magnetic simulations. We employ the plasma simulation code VORPAL [4] and focus on the proton and electron phase-space distribution at the rear side of the target. The lack of knowledge about the thickness of hydrogen-rich contamination layer requires a detailed parameter study, which has been done in 1D. In this work we investigate the expansion and divergence of a thick proton layer from the rear side of the target using 2D simulations. In order to make sure that the results are physically correct and reliable we performed a detailed convergence study over the grid size and macro-particle charge.

NUMERICAL HEATING IN 2D PIC SIMULATIONS

As we know, in 1D it is really easy to resolve the physical scale lengths (Debye-length) and we can use many macro-particles per cell in order to get better statistics and smoother plasma density. With resolution high enough we obtain results comparable to the fluid-hybrid codes, but the PIC code always gives us more data and realistic velocity phase-space distribution of particles. Therefore the PIC simulations are used to get insight into the smallest details of physical processes in plasma physiscs.

Very often in 2D we can not use the same high resolution. Because of the discretization of space and time we always have to be aware of the numerical errors which occur during field calculations and integration of equation of motion of particles. These errors can lead to increasing field amplitudes, consequently artificial particle acceleration. The main equations which are solved in the loop of a PIC code are the Faraday's and Ampere-Maxwell law:

$$\frac{\partial B}{\partial t} = -c\nabla \times E \tag{1}$$

$$\frac{\partial E}{\partial t} = c\nabla \times B - J \tag{2}$$

These equations are solved in the frequency domain by calculating the Fourier transform of the fields and then they are transormed back, because the equation of motion is integrated in the time domain. This additional step speeds up the calculations significantly. Due to the granulated representation of the density, the Fourier transform of J can contain very high frequencies, which can not be resolved by the spatial grid. The high frequency noise can be reduced by increasing the grid resolution or increasing the number of particle per cell (PPC). However these two options are very expensive in terms of computing power and CPU time. A much better method is the implementation of higher order particle shapes and field interpolation which will smooth out the fields and current density in the simulation. Thus the noise disappears and the simulation will be more stable with correct energy conservation, but it does not mean that result is closer to the reality or that it is more reliable [5]. Very often the high frequency modulation of the density has a physical reason and in this case we exclude a part of the physical processes by applying a smoothing technique.

Interaction of high intensity laser with over-dense plasma requires a very high number of grid-cells in order to resolve the very small cold electron Debye-length (λ_{Dc}). The usual length in both directions is a few tens of micrometers, while the Debye-length inside of the high density cold plasma is on the order of nanometers. In this case it is inevitable to use smoothing interpolations, which allows us the define grid cells larger than λ_{Dc}. In order to check the grid heating we performed several simulations with dense plasma (n_0=10^{27} m^{-3}) filling up completely the simulation box, which has periodic boundaries. The initial electron temperature was 1 keV. In Fig. 1 the simultaion results are shown for 4 different grid resolution. Two simulations were done with linear interpolation and particle shape, which results in a very strong heating of the electrons. This numerical effect is not present if we switch to the cubic (third order) smoothing even if the grid size is 40 times larger than λ_{Dc}. A weak heating can be observed only for very small PPC, brown line.

Another important effect which can increase the electron temperature is the numerical Cherenkov emission. It is related to the Courant criteria [6], which defines the time step for a stable simulation. Discretizing the space automatically leads to a dispersion relation which says that the phase velocity of electro-magnetic waves propagating on the grid is smaller than the speed of light. If we have high energy electrons in the system they can have velocity close to the speed of light which means that they can travel fatser than maximum phase velocity in the system. This situation results in the same effect what we observ in the reality: radiation into the medium. The emitted fields accelerate the electrons, thus their temperature is increasing. This effect

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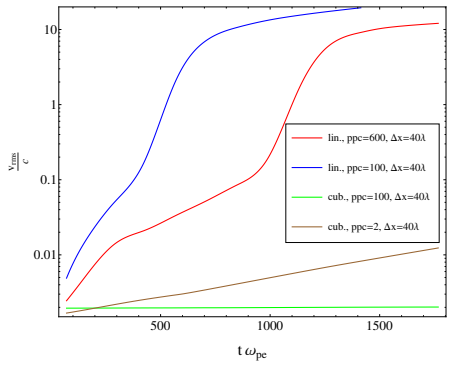

Figure 1: Normalized RMS momentum of elecrons for different simulation parameters. $\omega_{pe} = \sqrt{n_0 q_e^2/m_e\epsilon_0}$.

we can see in Fig. 2, where the black line shows that for this high resolution the grid heating is very small even with linear interpolation. The red line shows the result from the same simulation, but the electron temperature is relativistic and the blue line prooves again that the cubic interpolation suppresses the unvanted effect. In order to understand this we have to know that the Cherenkov emission is efficient for high wave numbers. For low frequencies it vanishes, that is why by eliminating the high frequency noise from the system we do not observe the heating.

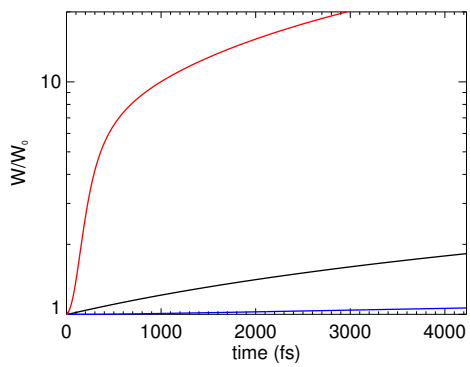

Figure 2: Total energy of the electrons over time in a simulation with $dx = 4\lambda_{Dc}$ and PPC=50. Legend: black - $T_h = 1$ keV, linear interp.; red - $T_h = 500$ keV, linear interp. and blue - $T_h = 500$ keV, cubic interp. ω_{pe}=1.78·10^{15} Hz.

SIMULATIONS INCLUDING THE LASER PULSE

In Fig. 3 the simulation setup is presented with specific boundary conditions. The simulation size is 50×50 μm and the target (red column) is at 7 μm from the left boundary. For this type of simulation the total energy of the system should be constant or slightly decreasing (due to the PML regions) after the laser pulse is off. It makes very easy to check if the grid heating is significant or not. The laser pulse duration was 200 fs and the peak intensity 6· 10^{23} W/m^2. The simulations were carried out with third order field interpolation and particle shape. The average CPU time of these simulations is 1 day and only 20 nodes were used.

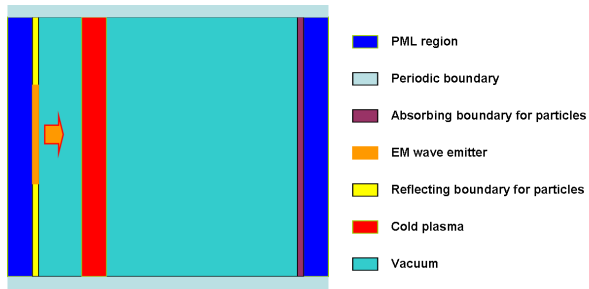

Figure 3: The simulation setup for a TNSA simulation.

The most important part of the laser ion acceleration via TNSA is the hot electron production. The electron heating up to relativistic temperatures happens on the fron side of the target and the laser skin depth (penetration depth, δ_E) becomes a crucial parameter. We found that the resulting hot electron temperature (T_h) is very sensitive on the grid resolution, because if δ_E is not well resolved then the energy absorption from the laser is not correct. Unfortunatelly this length is approximatelly 10 times λ_{Dc}, therefore the grid size should not be larger than this. It will reduce strongly our freedom in choosing the grid size. Choosing PPC is more related to the rear side of the target, where the plasma expansion happens. The simulations and an isothermal model [7] show that the expanding plasma has an exponential density profile in longitudinal direction and the density at the proton front decreases in time as $\sim 1/t^2$. If we want to resolve the density we have to use a very high PPC ($\approx$ 100 or more) which makes the simulation very slow. Anyhow we are interested in a very short time window: 200-300 fs, which is enough to understand and model the 2D expansion of a thick proton layer. In the case of the thin layer the grid size should be equal to the layer thickness, which can be smaller than λ_{Dc}. Therefore our 2D study has not been extended yet to this regime.

In order to check the effect of the grid resolution on the results we performed several simulations with different grid size and PPC. In Fig. 4 the results from simulations with the same PPC are shown. As we can see by changing the grid size the T_h is affected significantly and it does not converges yet. It is important to mention that the grid heating does not appear in any of the simulations, because the total energy is constant after the laser pulse, see fig. right. In Fig. 5 we keep the grid size constant and increase the PPC. Here a more clear convergence can be observed in the proton fron velocity and the T_h starts from the same value. An interesting feature is noticeable in the time evolution of energy: the remaining field energy (total minus particle energy) is larger if the PPC is smaller. The reason is that for large macro-charge the charge separation results

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in a higher field at the proton front. With other words the energy goes into the electric field, it is not transfered to the protons.

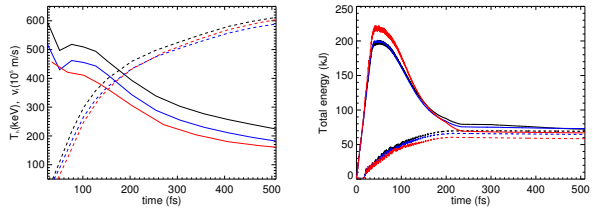

Figure 4: Left: Hot electron temperature (full line) and proton front velocity (dashed line). Right: Total energy in the system (full line) and total energy of all particles (dashed line). The color legend for both: $dx = 5\lambda_{Dc}$ (black), $dx = 10\lambda_{Dc}$ (blue) and $dx = 20\lambda_{Dc}$ (red). PPC=50.

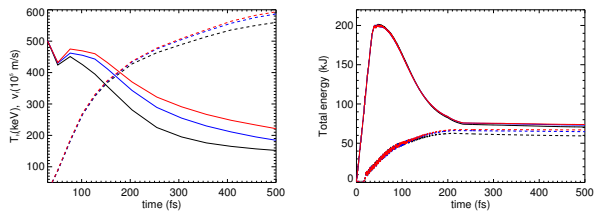

Figure 5: The same physiscal quantites as in Fig. 4. The color legend for both: PPC=20 (black), PPC=50 (blue) and PPC=100 (red). $dx = 10\lambda_{Dc}$.

After making sure that our simulations are correct we can study the physics of the two-dimensional plasma expansion. The used simulation parameters: $dx = 10\lambda_{Dc}$ and PPC=50. The only remaining issue is the hot electron temperature, which does not have its correct value at this resolution. This we do not consider a problem because by modelling the plasma expansion we take the hot electron parameters (measured temperature and density) from the simulation. Before we present the model we have to mention that in the next section non-periodic boundaries were used in the transverse direction. For the fields we used PML regions, just like in the longitudinal direction, and for the particles the so-called diffuse boundaries, which reflects back the electrons with a given thermal velocity distribution. For the thermal speed of the reflected electrons we take the initial one (cold). In this way we can mimic an infinite long transverse extension of the simulation box. With this trick we are closer to the reality, where the hot electrons spread out on the target surface and are replaced by cold electrons (return current), while the fields also disappear propagating in each direction.

ENVELOPE ANGLE OF THE PROTON BEAM

Our 2D simulations show that the hot electron density in transverse direction can be approximated with a Gaussian, which has a sigma (σ) comparable to sigma of the laser pulse and it increases slowly in time. Although the intensity profile is also Gaussian the hot electron temperature becomes isotrop in a few electron plasma periods, which is a very short time compared to the time scales of the expansion. Therefore we can assume a uniform temperature and just for sake of simpliciy we assume that it is contstant during the laser pulse. The peak value of the density (n_{h0}) is at the laser axis and it is measured from the simulation. One can calculate from the energy absorption, if it is known. We rely on the simulation and do not use other semi-empirical estimations to obtain the hot electron parameters. In the following x denotes the longitudinal and y the transverse direction.

After laying down the initial conditions and assumptions we can derive a transversal acceleration by using the results of P. Mora [7]. The model is based on the fact that electric field vector (E_y) which points into the transverse direction is proportional to the tangent of the surface angle which is determined by the proton front surface. As a simplification we calculate E_y just by multiplying E_x with the surface angle, because it is a small value and the electric field is always perpendicular to the surface. All we need to know is the time-dependent derivative of the proron front as a function of y. The starting equation gives the position of the ion front:

$$x_f(y,t) = 2\eta(y)t[\ln(\eta(y)t + \sqrt{(\eta(y)t)^2+2}) - \ln(\sqrt{2})] - 2(\sqrt{(\eta(y)t)^2+2} - \sqrt{2}) \quad (3)$$

where $\eta = \sqrt{n_h(y)/n_{h0}}$ and $n_h(y) = n_{h0}\exp(-y^2/2)$. Here y is normalized to σ, the time t is normalized to $1/\omega_{p0}$ and the longitudinal coordinate x is measured in the units of λ_{D0}, where $\omega_{p0} = \sqrt{n_{h0}q_e^2/m_p\epsilon_0}$, $\lambda_{D0} = \sqrt{T_h/m_p}/\omega_{p0}$. We have to mention that the Euler number is missing from the expression, because Mora derived the model for one-temperature model, but in the two-temperature case φ_0 appears in the exponent. It depends on the hot-to cold electron pressure ratio [8], also on y, which would make the equations way more complicated. Assuming that the cold electron density is much higher than the hot one, we can use the approximation $\varphi_0 \approx 0$ and $e^{\varphi_0} = 1$. If we calculate $\partial x_f/\partial y$, we get the following envelope angle:

$$\alpha(y,t) = -\frac{yt}{\Sigma}\left(\sqrt{\frac{1}{k(y,t)}} - \sqrt{1+\frac{1}{k(y,t)}}\right) \quad (4)$$

where $k(y,t) = \exp(-y^2/2)t^2/2$ and $\Sigma = \sigma/\lambda_{D0}$. Now we can simply say that $E_y(y,t) = \alpha(y,t)\cdot E_x(y,t)$, where [7]

$$E_x(y,t) = \frac{2\eta(y)}{\sqrt{2+\eta(y)^2t^2}} \quad (5)$$

The v_y of the protons at the front can be calculated if we integrate $E_y(y,t)$ over time, but it can not be done analytically. A very rough approximation gives us an analytical

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expression: $v_y(y,t) = v_x(y,t)\alpha(y,t)$, where v_x is the time derivative of Eq. 3. However we found that the exact solution is always roughly 3.3 times smaller than the analytical expression. Thanks to this interesting observation we have a very simple function which predicts the transverse velocity of the protons:

$$v_y(y,t) = v_x(y,t)\alpha(y,t)/3.3 \quad (6)$$

The next step is the validation of our simple model with correct PIC simulations. For this we compare the result of one simulation with the analytical predicitions. The parameters of the laser: τ =500 fs, I_L=0.8·10^{23} W/m^2 and σ_L=8.5 μm. The hot electron density and temperature were measured at the peak intensity of the laser and the corresponding normalization quantities: $\lambda_{D0} = 6.51 \cdot 10^{-8}$ m and $\omega_{p0} = 8.09 \cdot 10^{13} s^{-1}$.

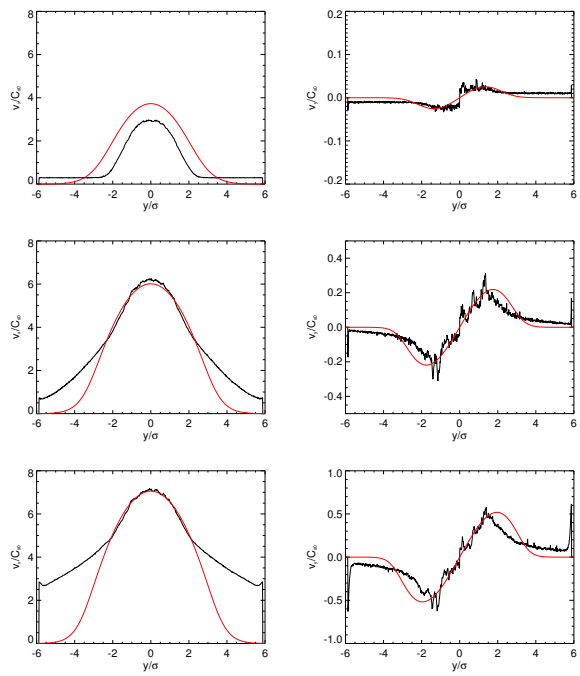

Figure 6: Longitudinal (left column) and transversal (right column) velocities of the proton front at the time moments: 80 fs ($\omega_{p0}t$ = 6.4, top row), 200 fs ($\omega_{p0}t$ = 16, middle row) and 320 fs ($\omega_{p0}t$ = 25.6, bottom row).

In Fig. 6 the comparison is presented for different time moments. As we can see the longitudinal velocity does not match with the model at the beginning because the T_h and n_{h0} did not reach yet their saturation value. The sigma used in the model was $\sigma = 8\mu$m. The transverse velocity fits quite well, but only close to the top of protons front. Farther from the center the hot electron density does not follow the gaussian shape, it is hagher than the one assumed in the model. The reason is that in 2D the particles can move only in two transversal directions, but in the reality they spread out in each direction and the density is proportional to $1/r$, where r is the radius (distance from the center). It means that the plasma expansion has a cylindrical simmetry, which can not be handled in our 2D planar simmetry. The consequence is that the electric field is trong also far from the axis of simmetry of the laser pulse and the proton front surface will be different from the one predicted by the model. Therefore the surface angle becomes smaller and the transverse field weaker. This is why we see smaller v_y in the simullation at the distances larger than 2σ. This effect can be seen in Fig. 7, where we compare the electric fields from 2D and 3D simulations. Other simulations show that the distortion of the front surface becomes stronger if the Σ is smaller, but our model is deduced for large laser spots, where the surface angle is still small.

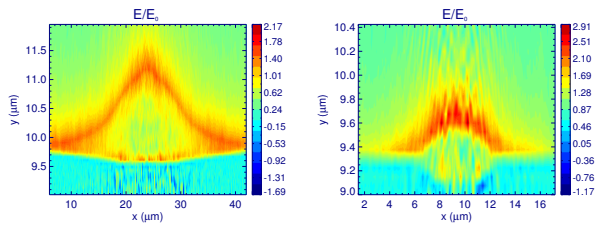

Figure 7: Contour plots of the longitudinal electric field in a 2D (left) and 3D (right) simulation. $E_0 = 1$ TV.

CONCLUSIONS

We could find the optimal numerical parameters for a 2D TNSA simulation, which ensures that the results are correct if the simulation is not too long. This type of simulations can be preformed with limited computing resources as well. The hot electron temeprature does not converege yet for our parameters, because the laser-plasma interaction has very small scale length and it is a complicated stochastic process which is difficult to resolve spatially. We have to rely on our measured values from the simulation and use them as input parameters in the plasma expasnion model. The model, derived in this contribution, is valid for large hot spots and for relatively short time (200-300 fs), but in principle it can be used as initial condition for other simulations where the grid size is much larger and the investigation of proton and electron velocity phase-space on a longer time scale is possible. The full description of the proton distribution is currently ongoing work, but it seems to be possible by using the presented model.

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