TNSA proton maximum energy laws for 2D and 3D PIC simulations

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Our virtual laboratory



Apart from jasmine, all of our codes are now free (GPL v3)

webpage: https://github.com/ALaDyn

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2D-3D PIC sims and laws

Since ALaDyn became open source¹, almost one year ago, we released these updates:

- Ported ALaDyn to the new Marconi HPC system deployed at CINECA (both the A1 and A2 partition)
- Rewrote the gaseous and solid target specifications and implementations, to ease simulations for recent experiments
- PWFA: new bunch shapes
- Deprecated the previous toolchain, ported everything to CMake
- Rewrote the I/O module to work around machine-level bugs on Marconi
- Add compatibility with old-ALaDyn input files
- Usual bugfixes

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¹we still have a version in-house a little bit different, we will release all the modules step-by-step

A consolidated regime TNSA energy spectrum

TNSA has a very well known energy spectrum, based on an exponential distribution with a precise cut-off energy E_{max} (*T* is the proton temperature).

$$\begin{cases} dN/dE = (E_{\text{max}}/T) \ e^{-E/T} & \text{for } E < E_{\text{max}} \\ dN/dE = 0 & \text{for } E > E_{\text{max}} \end{cases}$$



- laser pulse duration: $\tau = 40$ fs
- $\lambda = 0.8 \,\mu \text{m}$, P-polarized
- $I = 2 \cdot 10^{19} \text{ W/cm}^2, a_0 = 3$
- waist 6.2 $\mu {\rm m}$
- target: uniform Al foil, thickness $0.5\mu m \le L \le 8\mu m$
- \bullet contaminants: layer of H on the rear (non illuminated) side, fixed thickness $0.08 \mu {\rm m}$
- ionization level: fixed, Al⁹⁺, H⁺
- electron densities: $n_e^{Al} = 100 n_c, n_e^H = 10 n_c.$
- neglected preplasma (the temporal contrast is assumed as infinite)

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The problem Numerical simulations



Figure 1: Maximum energy rise in time. Left: the 2D case, right: the 3D case.

In 2D PIC TNSA simulations, a monotonic rise of E_{max} with time is observed whereas in 3D a slow trend towards a possible saturation to an asymptotic value is usually observed.

Two EMPIRICAL laws for $E_{\max}(t)$

Work originated from Schreiber et al. model². The acceleration of protons (contaminants) is due to the positive surface charge created on the rear target, thanks to the electron escape.



Figure 2: Left: 3D case (charge on a disc of radius R). Right: 2D case (charge on a strip of infinite length).

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²Phys. Rev. Lett., 97:045005, Jul 2006

Laser pulse: propagates along the z axis

Hypothesis: electrostatic potential V which vanishes at z = 0, where a uniform charge density σ , within a disc of radius R, is located.

$$V(\zeta) = 2\pi R \,\sigma \left(\sqrt{1+\zeta^2} - \zeta - 1\right) \qquad \qquad \zeta = \frac{z}{R}$$

A particle initially at rest accelerates and the law of motion is obtained from energy conservation. Since V(0) = 0, we have

$$m\frac{v^2}{2} + eV(z) = 0 \qquad v = \dot{z}$$

so that

$$E_{\infty} = m \frac{v_{\infty}^2}{2} = 2\pi e R \sigma$$
 $v_{\infty} = \dot{z}(\infty)$

The kinetic energy of the particle, after integrating the equation of motion, is

$$E_{\rm kin}(t) \simeq E_{\infty} \left(1 - \frac{t^*}{t}\right)^2 \qquad t > t^* = \frac{R}{4v_{\infty}}$$

Since this is an asymptotic law, we may assume that E(t) = 0 for $t < t^*$.

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$$\begin{cases} E_{\max}^{(3D)}(ct) = 0 & \text{for } t < t^{*(3D)} \\ E_{\max}^{(3D)}(ct) = E_{\infty}^{(3D)} \left(1 - \frac{ct^{*(3D)}}{ct}\right)^2 & \text{for } t > t^{*(3D)} \end{cases}$$

We can perform a linear fit by defining $y = \sqrt{E}$ and x = 1/ct, so that the previous law becomes

$$y = a + bx$$
 $E_{\infty}^{(3D)} = a^2$ $ct^{*(3D)} = -\frac{b}{a}$

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Laser pulse: propagates along the z axis

Hypothesis: electrostatic potential V which vanishes at z = 0, where a uniform charge density σ , on an infinite strip along the y axis and with a size R along the x axis, is located.

$$V(z) = 4R\sigma \left(-\zeta \arctan \frac{1}{\zeta} + \log \frac{1}{\sqrt{1+\zeta^2}}\right)$$
$$\simeq -4R\sigma \log(1+\zeta)$$

where we defined $\zeta = z/R$.

The potential in this case diverges logarithmically and consequently the particle accelerates indefinitely. We approximate the potential energy with

$$e\hat{V}(z) = -E_{\infty}\log(1+\zeta)$$

so that

$$E_{\infty} \equiv m \frac{v_{\infty}^2}{2} = 4eR\sigma$$

Integrating the equations of motion we have

$$E_{\rm kin}(t) = E_{\infty} \log\left(\frac{t}{t^*}\right)$$
 $t \ge t^* = \frac{R}{v_{\infty}}$

Since this is an asymptotic law, we may assume that E(t) = 0 for $t < t^*$.

$$\left\{ \begin{array}{ll} E_{\max}^{(2D)}(ct) = 0 & \text{for } t < t^{*(2D)} \\ E_{\max}^{(2D)}(ct) = E_{\infty}^{(2D)} \log \frac{ct}{ct^*} & \text{for } t > t^{*(2D)} \end{array} \right.$$

We perform a linear fit by defining y = E and $x = \log ct$, so that the previous law becomes

$$y = a + bx$$
 $E_{\infty}^{(2D)} = b$ $ct^{*(2D)} = e^{-a/b}$

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Results for 2D simulations

Normal incidence, different target thicknesses



Figure 3: Left: E_{max} versus ct, PIC simulation (symbols) vs fit (continuous line): blue $L = 0.5 \,\mu\text{m}$, green $L = 1 \,\mu\text{m}$, violet $L = 2 \,\mu\text{m}$, orange $L = 4 \,\mu\text{m}$, black $L = 8 \mu\text{m}$. Right: the same as the left panel but in a logarithmic scale for ct which clearly shows the linearity and the accuracy of the fit.

Results for 2D simulations

Non-normal incidence, fixed target thickness



Figure 4: Left: E_{max} versus ct, PIC simulation (symbols) vs fit (continuous line): $\alpha = 5^{\circ}$ green, $\alpha = 10^{\circ}$ violet and $\alpha = 15^{\circ}$ orange. Right: the same data are plotted as with a logarithmic scale for ct, which shows how the data stay on a line and the accuracy of the linear fit.

Results for 3D simulations

Normal incidence, different target thicknesses



Figure 5: Left: E_{max} versus ct, PIC simulation (symbols) vs fit (continuous line): $L = 0.5\mu$ m blue, $L = 1\mu$ m green and to $L = 2\mu$ m violet. Right: Plot of $\sqrt{E_{\text{max}}}$ versus 1/ct which shows their linearity and the accuracy of the fit.

Comparison with experiments

Where are we?



Figure 6: E_{max} versus L from various experiments ($a_0 \sim 3$ and a metal target): Ceccotti's (45° incidence angle) (blue), Neely's (30°) (green), Flacco's (45°) (violet), fits from our 2D PIC simulation at zero degree incidence (brown), fits from 2D sims at 30° incidence (red) and fits from 3D PIC simulation at zero degree incidence (black).

- The asymptotic value of the cut-off energy of protons, which is what is measured in experiments, is difficult to extract from PIC simulations
- The 2D results do not exhibit a saturation
- The 3D results show that a saturation might be reached, despite at a large time ($ct > 200 \,\mu$ m), which is computationally too expensive

- We formulated two empirical laws for 2D and 3D simulations, which depend on the asymptotic energy E_{∞}
- The fits to the 2D and 3D results coming from PIC simulations are quite good and the statistical uncertainties are a few percent
- The extrapolated values E_{∞}^{2D} and E_{∞}^{3D} are comparable
- E_{∞}^{2D} and E_{∞}^{3D} can be fully calculated fitting the results obtained before $ct \leq 50 \sim 60 \,\mu\text{m}$, which is a distance reachable also in 3D simulations

- The fitting appears to be satisfactory also for small incidence angles, even though the model was developed for normal incidence
- The proposed phenomenological model is adequate to avoid the arbitrariness in the choice of the time at which the asymptotic cut-off energy is chosen in numerical simulations
- 2D simulations may have a quantitative value, with an adequate extrapolation, rather than being of purely qualitative nature