Numerical and theoretical modelling of plasma-based acceleration schemes

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Pisa, 14/03/2019

Outline

1. Introduction & Motivations
2. Plasma physics
   - Laser-Plasma interaction
   - Linear regime
   - Nonlinear regime
3. Plasma simulations
   - Particle-In-Cell numerical scheme
   - An example of reduced model: the envelope approximation
4. Applications
   - Innovative acceleration scheme for high quality electron bunch
   - Application of the numerical methods for the scheme validation
   - Results

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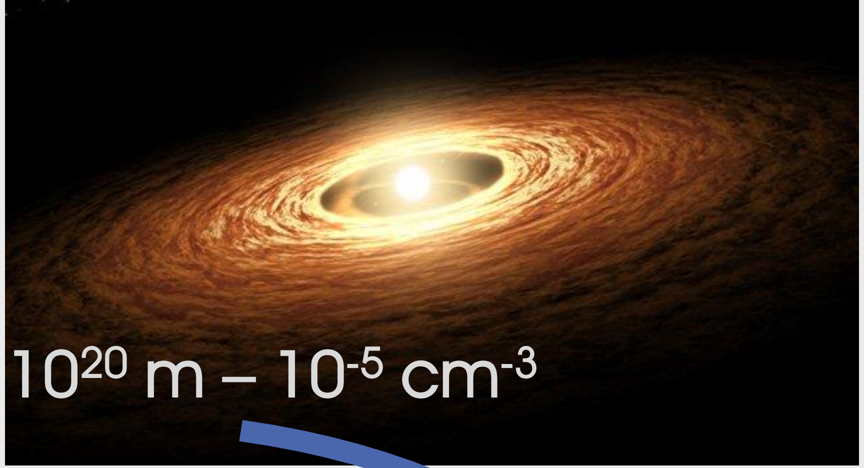
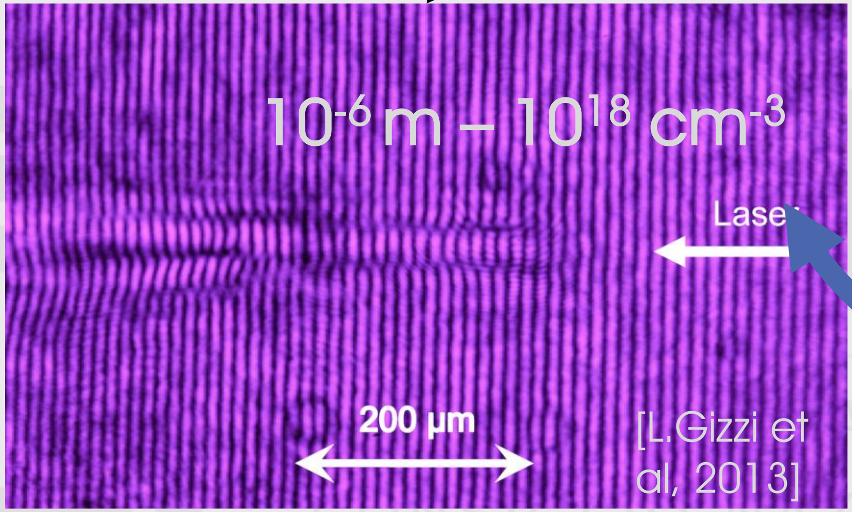
What is a Plasma?

- Ionized gas in which positive and negative particles are free to move with respect to each other
- Composes most of the known matter in the universe
- Particles present collective behaviour
- Can sustain ultra-large electric and magnetic fields

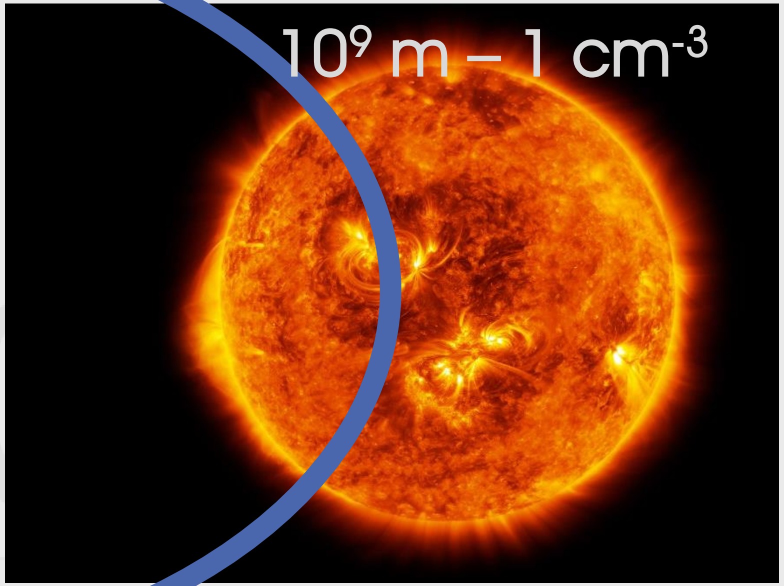
Typical density, temperature and length scale

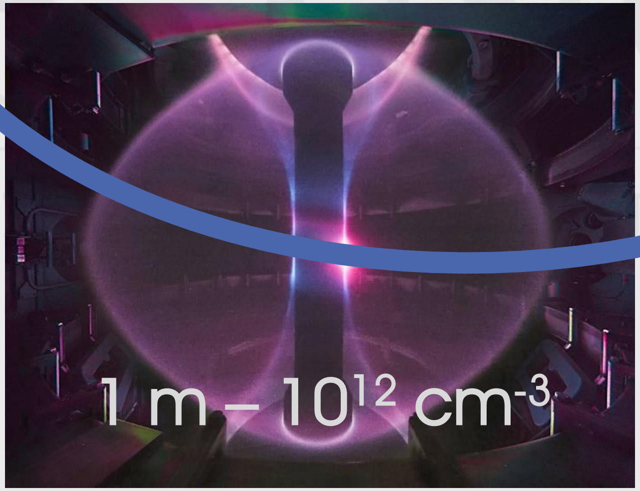


We work here: laboratory plasmas for acceleration



Unique theory of plasma spanning every range: unfeasible





Plasma acceleration: the new frontier

Plasma acceleration [Tajima, Dawson, 1979]

Plasma waves can reach electric fields up to order of magnitude larger than the breakdown fields of the radio frequency cavities

Laser driven ← Self/External injection → Beam driven

Laser driven

Pros
- Highly tunable
- Accelerated bunch can be created from scratch
- Light can be guided

Cons
- Pulse diffraction
- Bunch quality (emittance, energy spread, stability)

Beam driven

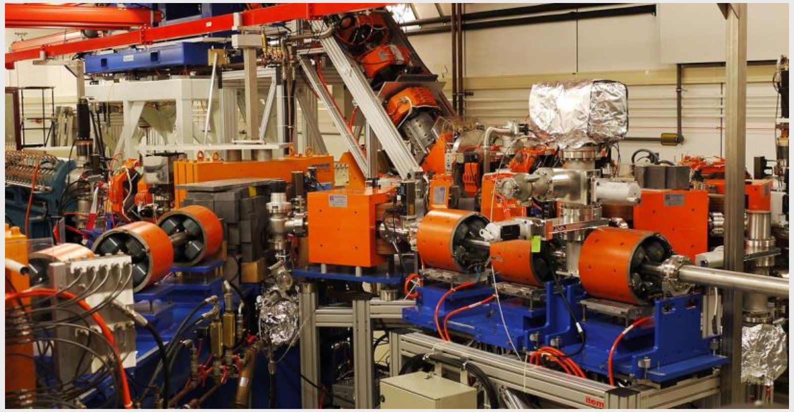
Pros
- Longer acceleration distances
- Does not suffer for diffraction

Cons
- External accelerated beam needed
- Beamline is needed to guide driver

Production of a 4.2 GeV electron beam in a 9 cm plasma channel
[Leemans, Nagler, Gonsalves et al., *Nature* 2006, Leemans, Gonsalves, Mao et al., *PRL*, 2014]

Conventional acceleration

Can we reach comparable energies and shirink their size?



- Need higher and higher energies to explore region near the «unification of forces»
- Reached considerable (and probably impassable) size

- Free Electron Lasers (FEL) need low energy spread accelerated beams
- ILC (Japan?) is being downgraded due to its extreme cost
- FCC concept study submitted Jan 2019. 24B€ and 100 Km circumference

Laser and plasma regimes

Plasma

- Obtained by preionizing pulses
- Density must be controllable and allow high energy gains
  $n \sim 10^{16\text{-}19}$ cm^{-3}
- Initially uniform and neutral, usually Hydrogen like
- Plasma wavelength $\sim$1-100 μm
- Total accelerating length L$\sim$10-100 cm

Incoming driver

Electron

Laser

- Power $\sim 10^{12\text{-}15}$ W
- Pulse energy $\sim$ 1 J
- Pulse duration resonant with plasma wavelength, t$\sim$100 fs → CPA technique for ultra-short pulses:
- Laser wavelength $\sim$ 1 μm (e.g. Ti:Sa 0.8 μm)
- Laser waist w$\sim$10-100 μm, depending on the acceleration regime one wants to exploit

Physics Nobel prize 2018

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Laser – Plasma interaction

Set of equations governing the laser-plasma interaction, written in normalized units

$$\begin{cases} \frac{1}{c}\frac{\partial}{\partial t}n + \nabla\cdot\left(\frac{\mathbf{u}}{\gamma}n\right) = 0 \\ \frac{1}{c}\frac{d}{dt}(\mathbf{u}-\mathbf{a}) = -\frac{1}{2}\nabla\left(\frac{\mathbf{u}}{\gamma}\cdot\mathbf{a}\right) + \nabla\phi \\ \nabla^2\phi = k_p^2 n \\ \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{a} - \nabla^2\mathbf{a} + \frac{1}{c}\frac{\partial}{\partial t}\nabla\phi = -k_p^2 n\frac{\mathbf{u}}{\gamma} \end{cases}$$

$$\mathbf{a} = \frac{e\mathbf{A}}{mc^2} \quad \phi = \frac{e\Phi}{mc^2} \quad \mathbf{u} = \frac{\mathbf{p}}{mc} \quad n = \frac{n_e}{n_0} \quad k_p = \frac{\omega_p}{c}$$

No general analytical solution: intrinsic nonlinearities due to the E.M. and plasma coupling

- Linearization $\mathbf{a} \ll 1$
- Broad pulse (1D) $\nabla_\perp \sim 0$

Conservation of canonical momentum: $\mathbf{u}_\perp = \mathbf{a}_\perp$ → Laser **strenght** determines the motion regime

$\mathbf{a}_\perp \ll 1 \rightarrow \mathbf{p} \ll mc$ Linear (classical)

$\mathbf{a}_\perp \sim 1 \rightarrow \mathbf{p} \sim mc$ Nonlinear

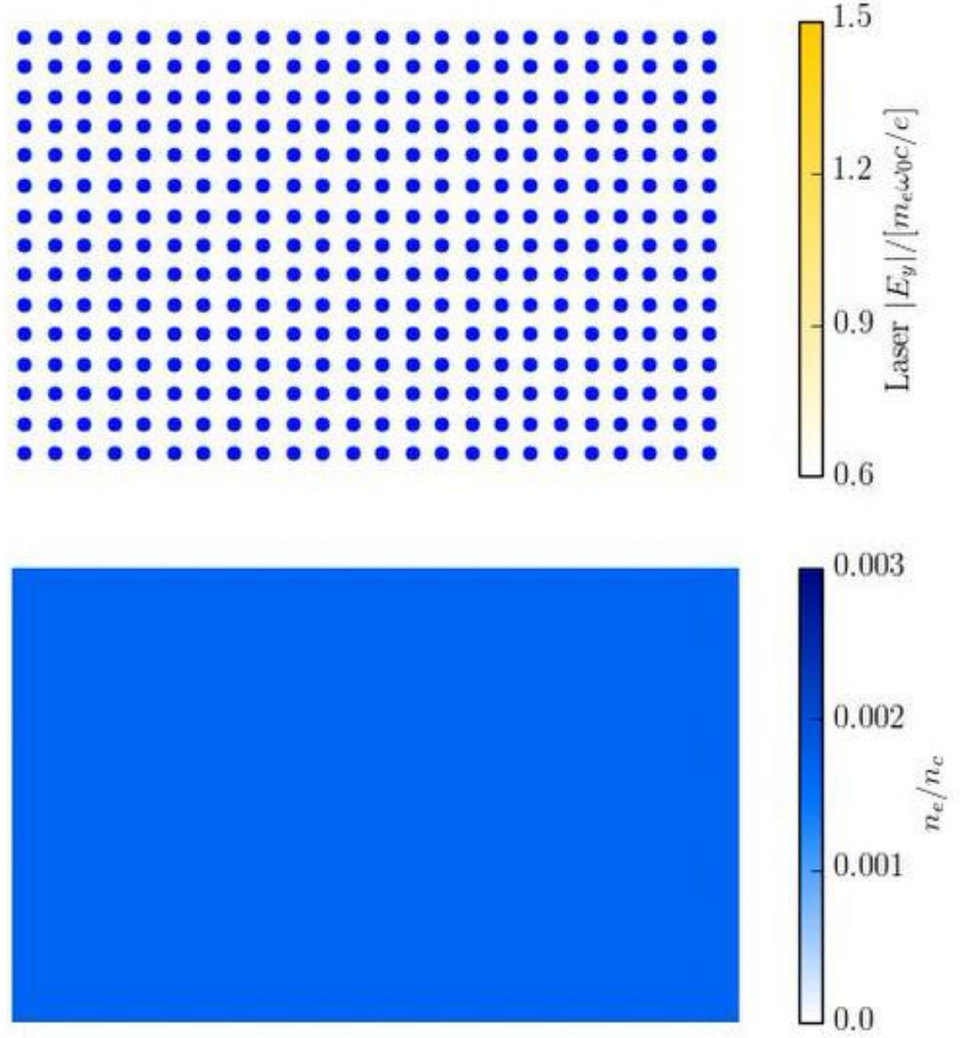
$\mathbf{a}_\perp \gg 1 \rightarrow \mathbf{p} \gg mc$ Strongly nonlinear (relativistic)

Example of a wakefield excitation

TOP: electron (blue) and ion (red) motion induced by the laser passage. Laser field is yellow

- Laser pulse travelling from left to right
- Pulse duration resonant with plasma frequency
- Ponderomotive force displaces electrons and produces an electrostatic **wakefield**

Bottom: electron density resulting from the laser passage. Lighter regions are more depleted than darker ones



Courtesy of Francesco Massimo, LLR, Paris

Ponderomotive force

Strong E.M. field interacting with the plasma: **nonlinear effects**

Fluid momentum equation with vector potential $\longrightarrow$ $$\frac{d}{dt}\left(\mathbf{p} + \frac{q}{c}\mathbf{A}\right) = \frac{q}{2c}\nabla\left(\frac{\mathbf{p}}{m\gamma}\cdot\mathbf{A}\right)$$

Perturbative solution $\mathbf{p} = \mathbf{p}_1 + \mathbf{p}_2$

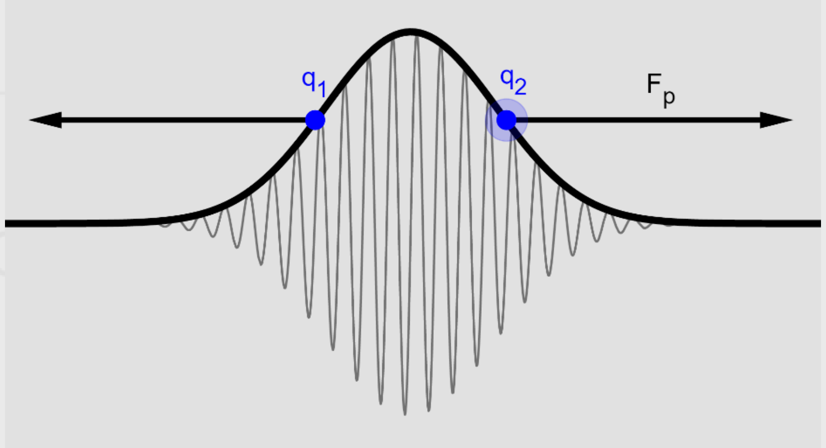
$$\frac{d}{dt}\left(\mathbf{p}_1 + \frac{q}{c}\mathbf{A}\right) = 0$$ Conservation of canonical momentum (plane wave)

$$\frac{d}{dt}\mathbf{p}_2 = -\frac{q^2}{2m\gamma c^2}\nabla\left|\mathbf{A}\right|^2$$ Nonlinear motion induced by the **envelope** of E.M. field (radiation pressure)

Radiation pushes particles from regions of high intensity to low intensity ones

APPLICATION: Laser pulse can excite plasma waves

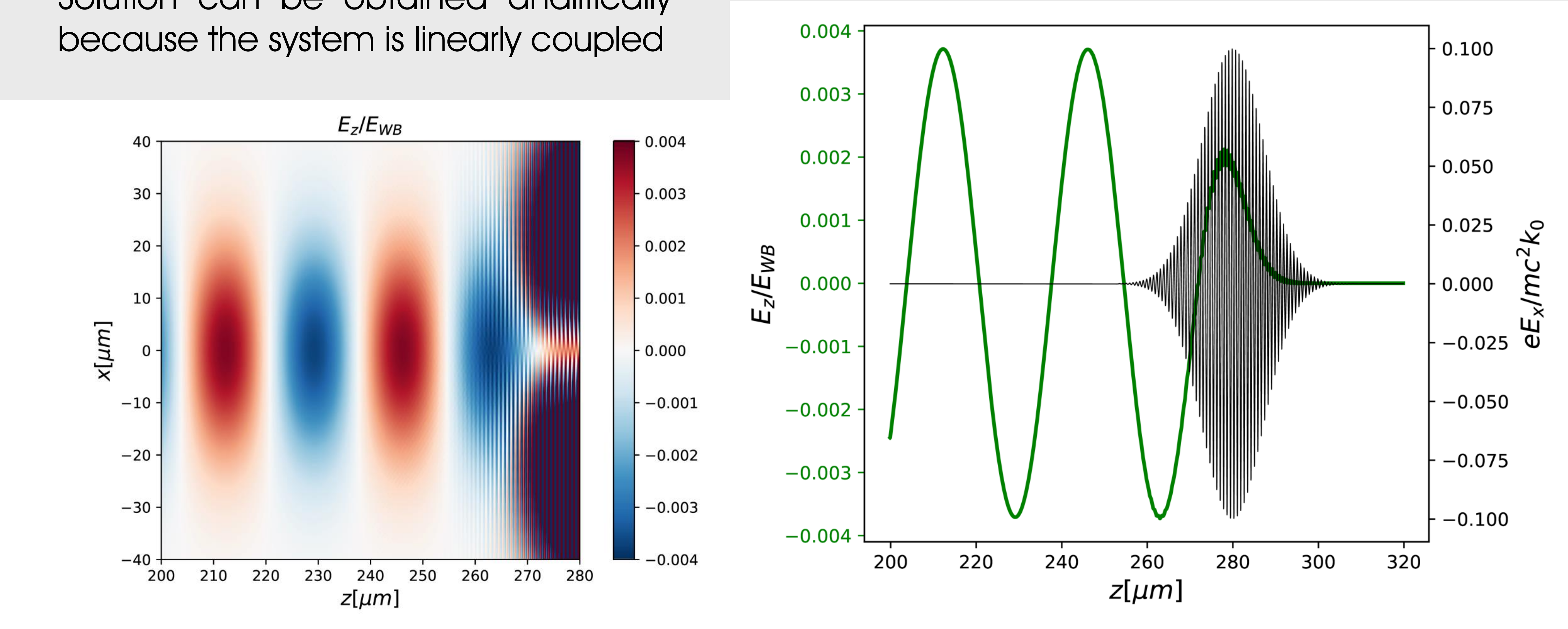
1. Laser pulse pushes particles
2. Plasma restores disclocated charges
3. Electrostatic wave is generated
4. Travelling pulse produces a wake



Linear regime

$$\mathbf{E} = -\frac{cE_{wb}}{2}\int_0^t \sin\left[\omega_p\left(t-t'\right)\right]\nabla\mathbf{a}^2 dt'$$

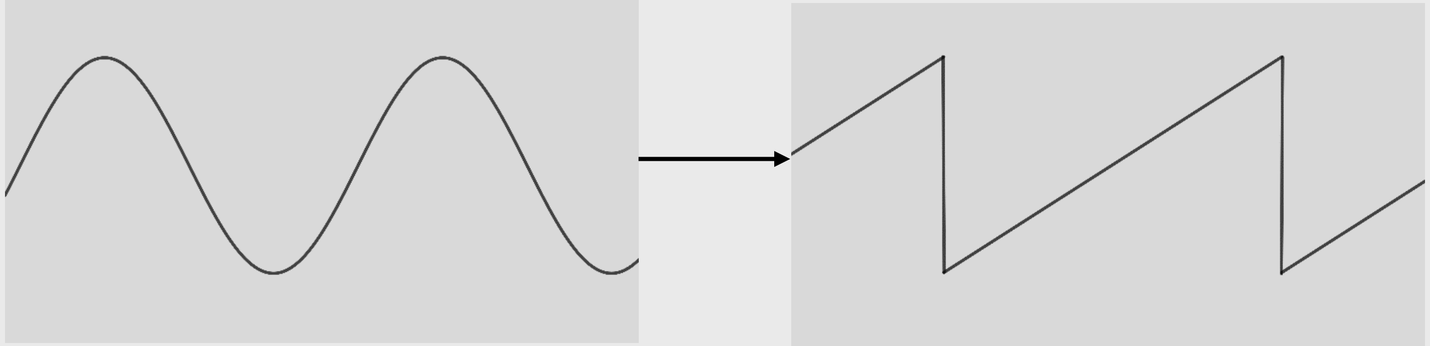
Solution can be obtained analitically because the system is linearly coupled



Nonlinear regime and wave breaking

If the perturbation is of the order of

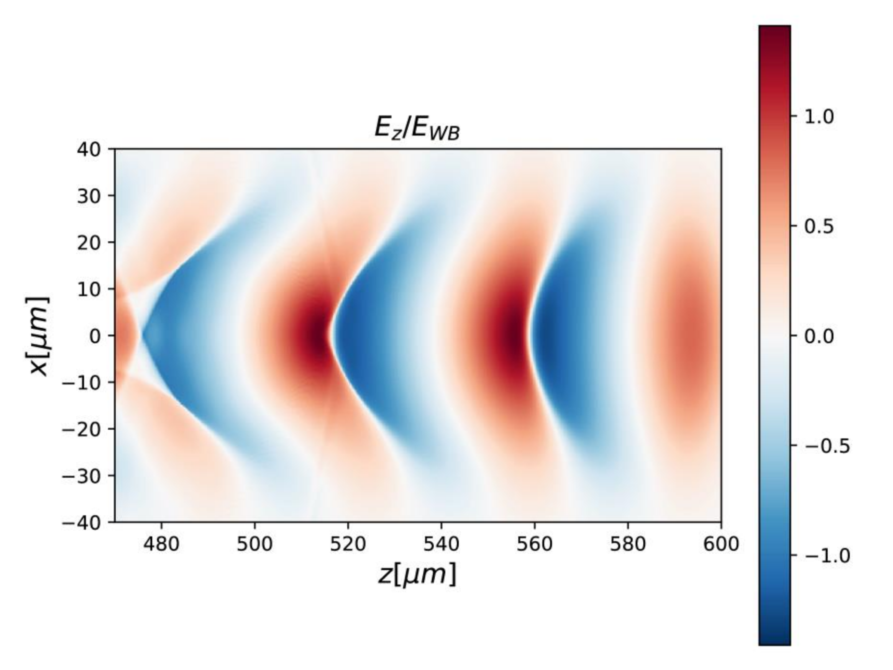
$$E_{wb} = \frac{m_e \omega_p c}{e}$$ [Dawson, *PR*, 1958]

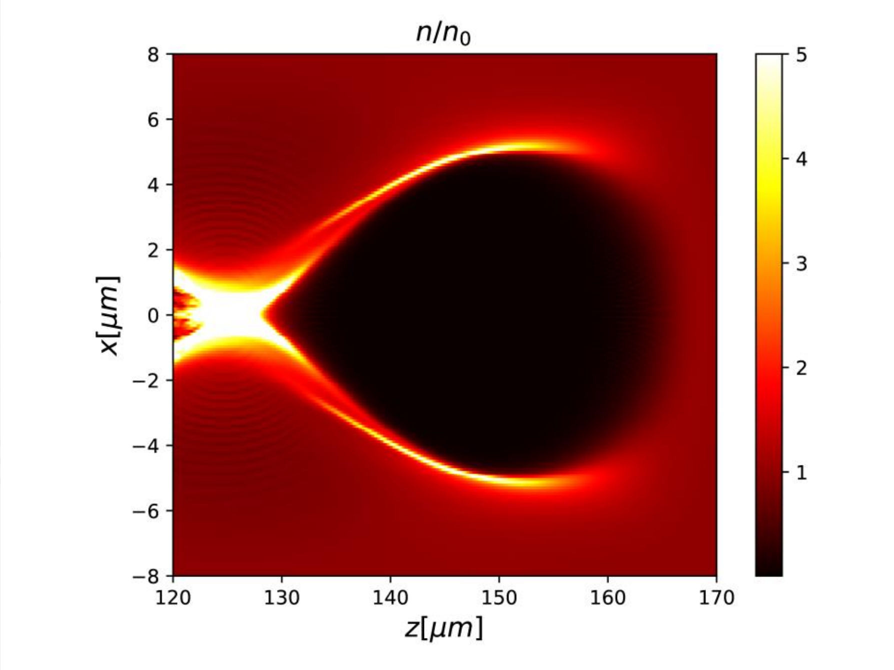


Electrostatic waves steepen up to the **wavebreaking**

$$E_{wb}\left[\frac{V}{cm}\right] \simeq 0.96\sqrt{n_0\,[cm^{-3}]}$$ → Accelerating fields up to 100 GV/m

Mildly relativistic





Plasma bubble (strong 3D correlation)

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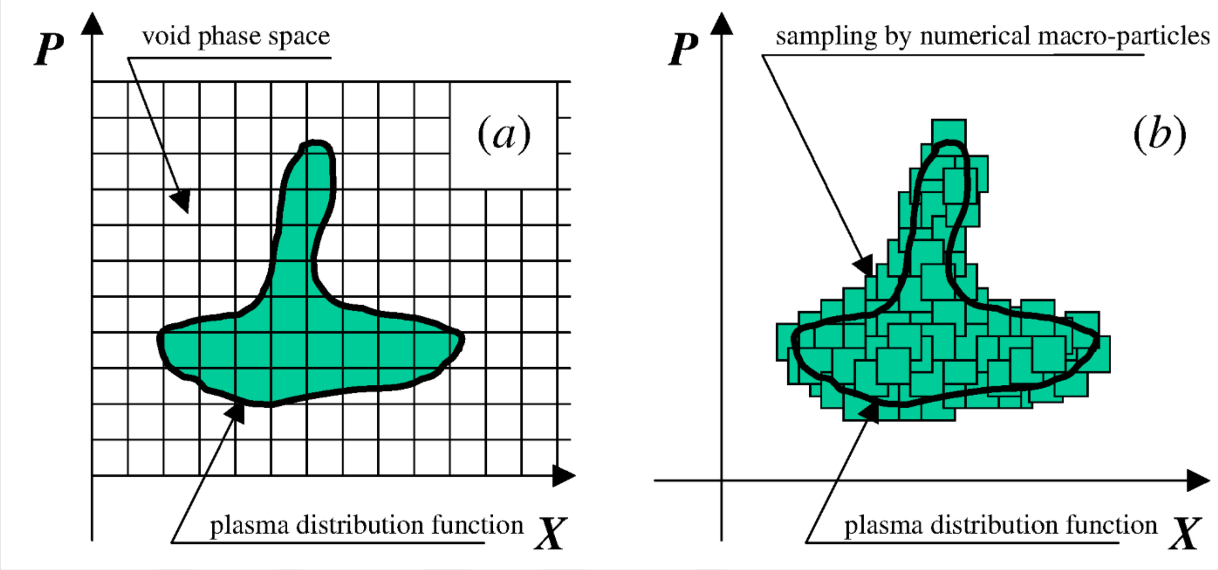
Particle-In-Cell

Numerical simulation are essential to investigate the fully nonlinear laser – plasma system

Vlasov eqution simulation:
unfeasible

$$\partial_t f_s + \frac{\mathbf{p}}{m_s} \cdot \nabla_{\mathbf{x}} f_s + \mathbf{F}_L \cdot \nabla_{\mathbf{p}} f_s = 0$$

$$F_L = q_s \left[\mathbf{E} + \frac{\mathbf{p}}{m_s c} \times \mathbf{B} \right]$$



Introduction of numerical macroparticle:
- Kinetic effects
- 3D space
- Local equations

Resolution of Klimontovich statistical formulation

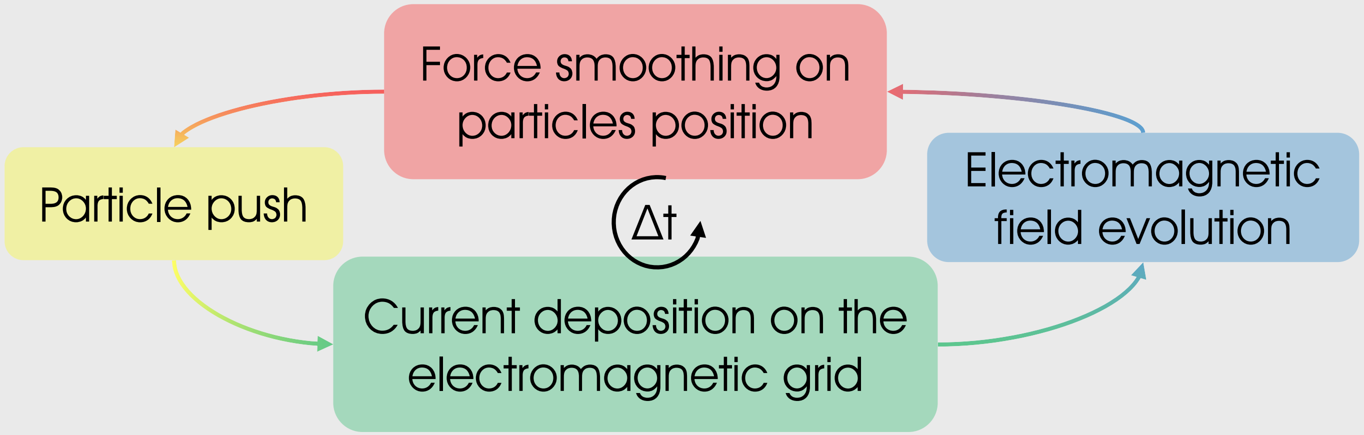
$$\dot{\mathbf{x}}_i = \frac{\mathbf{p}_i}{m\gamma}$$

$$\dot{\mathbf{p}}_i = q \left[\mathbf{E}(\mathbf{x}_i) + \frac{\mathbf{p}_i}{mc\gamma} \times \mathbf{B}(\mathbf{x}_i) \right]$$

$$\rho(\mathbf{x}, t) = qN \int f(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}$$

$$\mathbf{J}(\mathbf{x}, t) = qN \int \frac{\mathbf{p}}{m\gamma} f(\mathbf{x}, \mathbf{p}, t) d\mathbf{p}$$

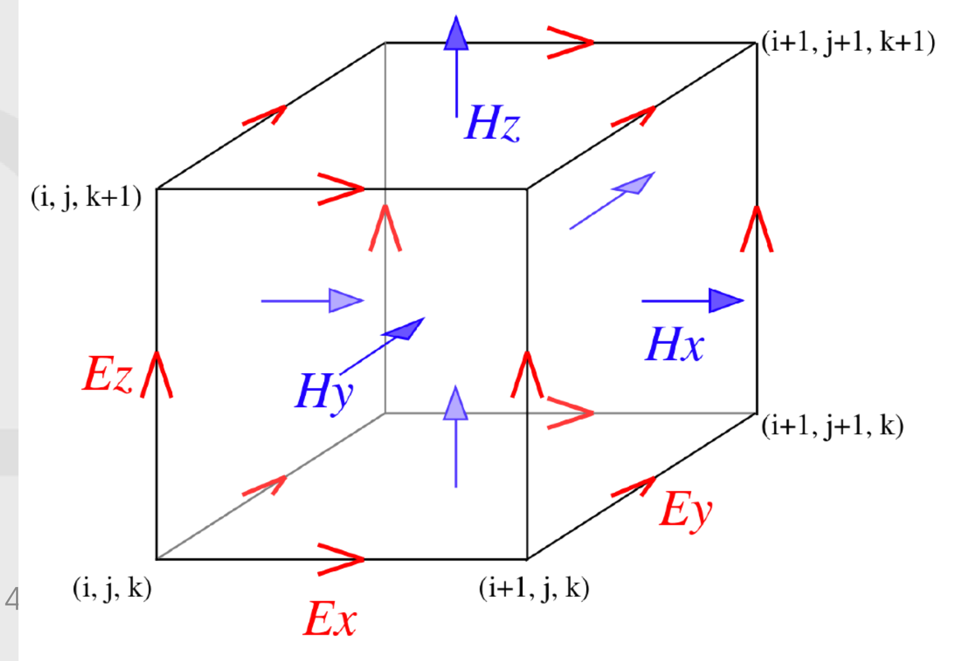
Selfconsistent loop of a PIC code



To obtain a fully selfconsistent particle field dynamics in an interval Δt

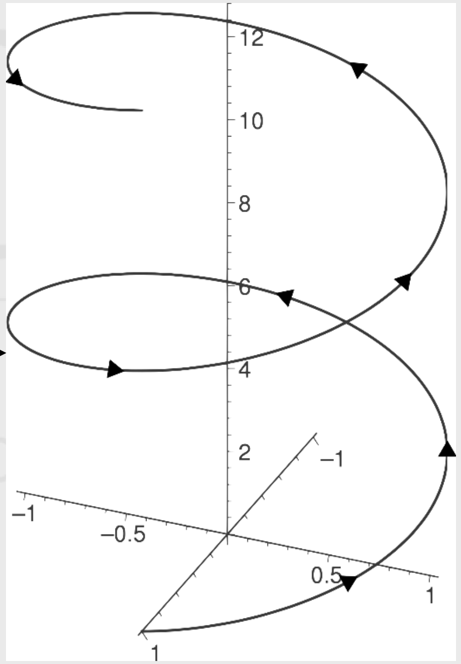
- Particle trajectory is computed
- Particle current and density are evaluated
- Electric and magnetic fields are evolved with given sources
- They determine a new force on the particles

E.M. evolution: **Yee scheme**



Particle – grid interaction: core of the PIC code

Spline functions



Trajectory: **Boris pusher** [Boris,1970]

Computational macroparticles

Macroparticles ⟶ Ensemble of physical particles

x – shape	p – shape
$b_n\left[\mathbf{x} - \mathbf{X}_i(t)\right]$	$\delta\left[\mathbf{p} - \mathbf{P}_i(t)\right]$

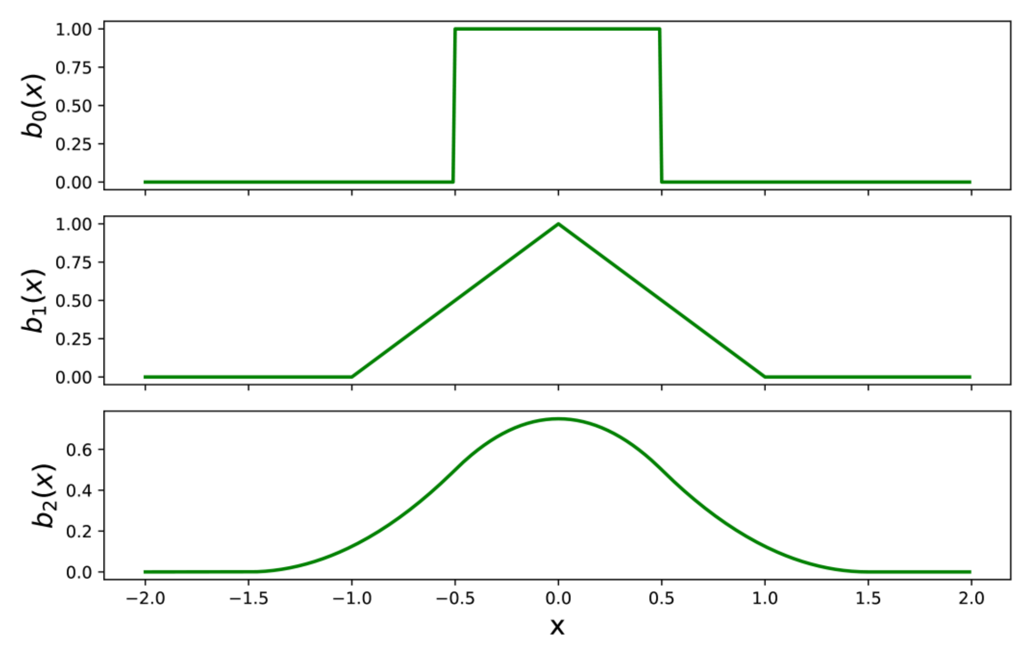
- Sample of the phase-space distribution function
- Evolve according the equation of motion
- Equations are equivalent to the Vlasov – Maxwell characteristics
- By smoothing macorparticles, distribution function at any time is obtained

Macroparticle spline: link between particles and grid

Spline for finite number of particles:
- Compact support
- Normalized
- At least cover one cell

#cells covered ⟷ Range of interaction

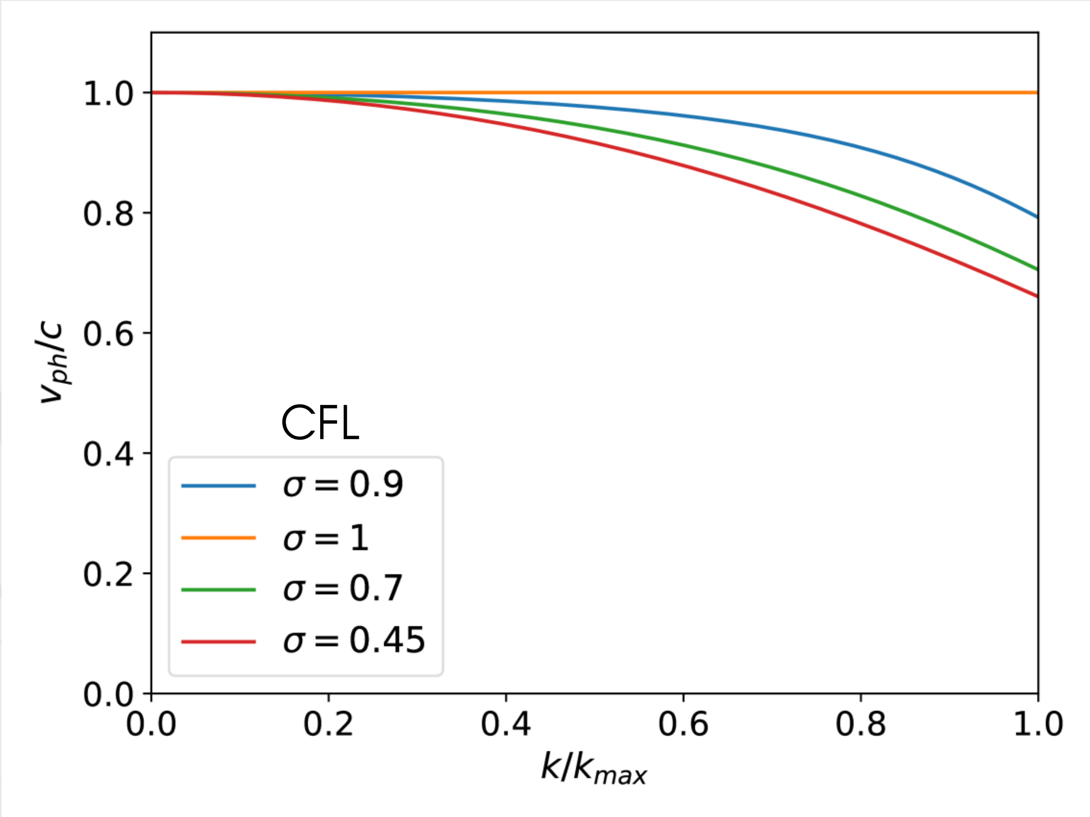
Not an N-body: unfeasible



Particle-In-Cell limitations

Even though they are powerful, PIC codes present some limitations

- Numerical dispersion of electromagnetic waves
- High computational cost due to the numer of particles
- Electron oscillations must be resolved: high resolution



High number of particles needed for statistical reasons: better sampling and smoothing

PIC retain all motion scales: disadvantageous on multi-scale systems or very long simulations $L_{tot} \gg \lambda_0$

Typical computational cost

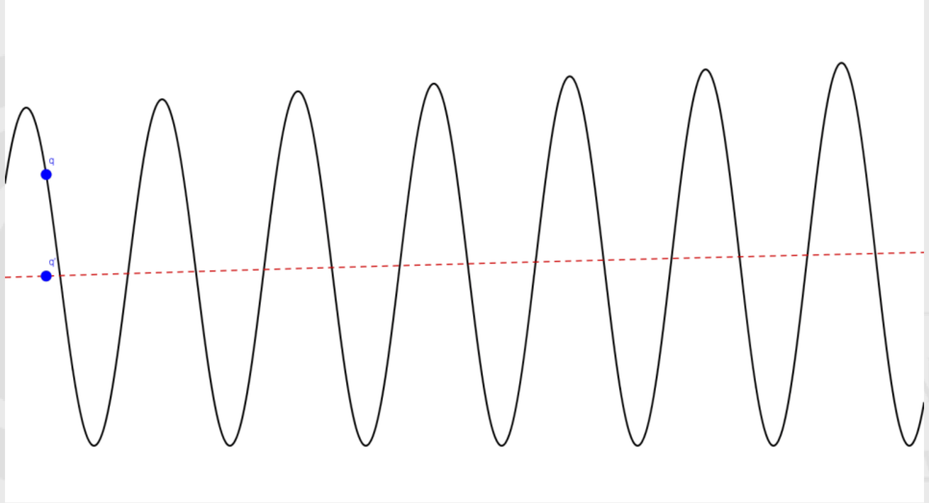
$$\lambda_0 \sim 1\mu\text{m}, \; L_{tot} \sim 5\text{cm} \rightarrow T_{tot} \sim Mh$$

Computational time

Reduced model: envelope approximation

Relevant scales much longer than the laser wavelength: no need to resolve wavelength, because the motion is coupled to the **laser envelope** length scales

We look for a way to describe a laser pulse evolution without resolving its wavelength → Reduced resolution in simulations equals a lot of time saving!



Consistent theory to:

- Adequately describe pulse envelope evolution
- Move particles retaining their averaged motion (no oscillations)
- Include the effects of the laser oscillation in the evolution equations

- Laser envelope
- Electric potential
- Density waves
- Electrostatic field

↔ Resonant with plasma frequency: **macroscopic motion**

$$k_p = \omega_p / c$$

System quickly damps fast oscillations outside laser pulse

Averaged particles dynamics

$$\frac{1}{c}\frac{d\mathbf{u}}{dt} = k_p\left[\mathbf{E}_w + \frac{\mathbf{u}}{\overline{\gamma}} \times \mathbf{B}_w\right] + \mathbf{F}_L$$

$$\frac{1}{c}\frac{d\mathbf{x}}{dt} = \frac{\mathbf{u}}{\overline{\gamma}}$$

$$\mathbf{F}_L = -\frac{1}{4\overline{\gamma}}\nabla\left|\hat{\mathbf{a}}\right|^2 \quad \overline{\gamma}^2 = 1 + \left|\overline{\mathbf{u}}\right|^2 + \frac{\left|\hat{\mathbf{a}}\right|^2}{2}$$

- Particle phase space evolves on **long** time scales
- Wake fields and laser pulse are two computationally different objects
- We define the average γ as the sum of the averaged terms

The ponderomotive force due to the laser pulse contributes separately → This is possible because we can split the sources

- Laser pulse: fast varying currents
- Wake fields: slow varying currents

Ponderomotive approximation

$$\overline{\gamma}^2 = 1 + \left|\overline{\mathbf{u}}\right|^2 + \frac{\left|\hat{\mathbf{a}}\right|^2}{2} \longleftarrow \overline{\gamma}(\mathbf{p},\mathbf{a}) = \gamma(\overline{\mathbf{p}},\hat{\mathbf{a}}) + \Delta$$

?? This in an *a priori* assumption
Empirical observations suggest this is a good approximation

Laser equation solver

1. Retains the second temporal derivative (full wave operator)
2. Solved in the LAB frame
3. The operator is inverted **explicitly**

$$\left[\partial_{t,t} - 2i\omega_0(\partial_t + c\partial_z) - c^2\nabla^2\right]\hat{\mathbf{a}} = -\omega_p^2\chi\hat{\mathbf{a}}$$

Second derivative is important for depleted pulses [Benedetti, Schroeder et al., *PFCF*, 2018] and regularizes the explicit inversion of the operator

Numerical evolution equation

$$\mathcal{D}_{t,t}a - 2i\omega_0\mathcal{D}_t a = \hat{S}\left[a\right]$$

→ Invert the formula by the means of centered derivatives

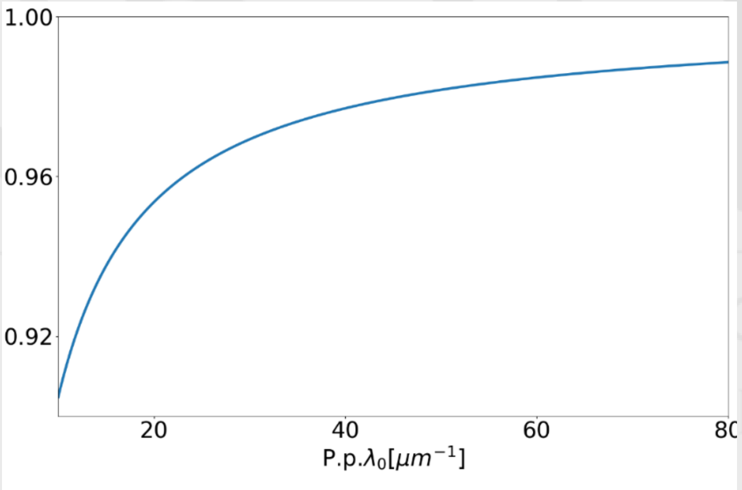
Explicit advancement

$$a^{n+1} = F\left(a^n, a^{n-1}\right)$$

Stability

CFL $\sigma \simeq \sqrt{1 - \frac{k_0\Delta x}{2\sqrt{N_d}}}$

[Terzani, Londrillo, *CPC*, 2018 submitted]



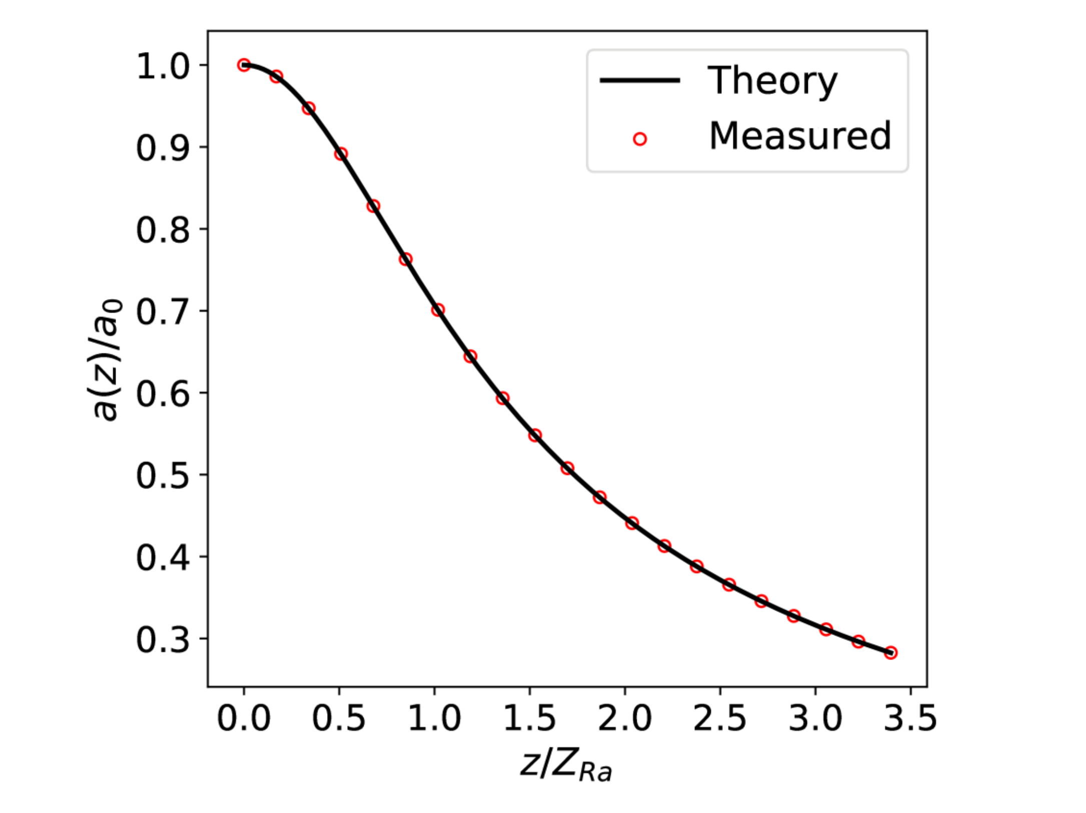
The lab frame is chosen for consistency reasons with the rest of **ALaDyn** and to be able to perform an explicit inversion

Explicit inversion is faster than the implicit one and guarantees the same CFL (stability) condition of a standard PIC

Benchmark against the theoretical results

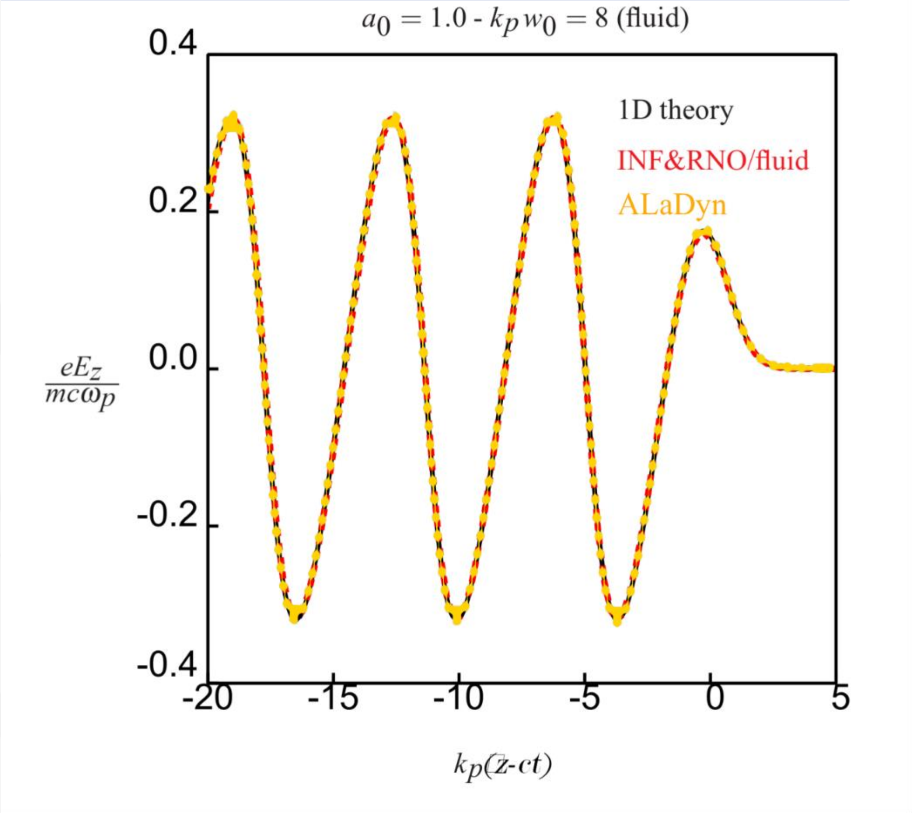
Rayleigh diffraction in vacuum

Verified correctness of laser solver



Longitudinal electric field in 1D approximation

Verified correctness of particle pusher



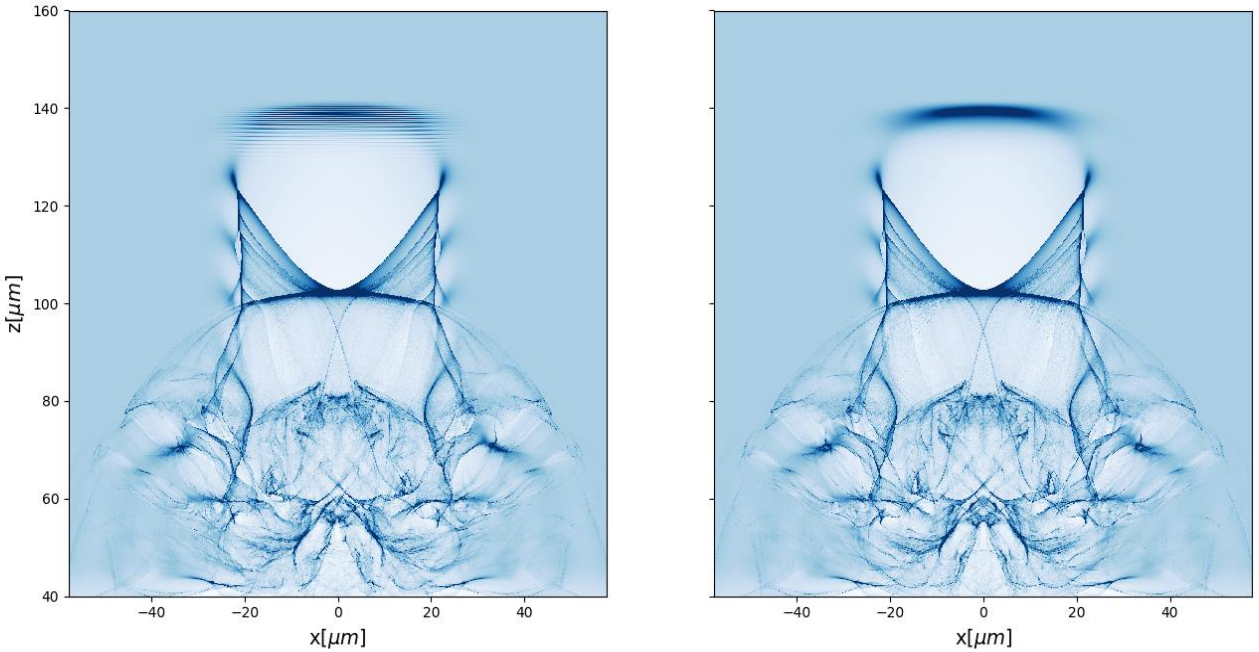
Benchmark against fully PIC simulations

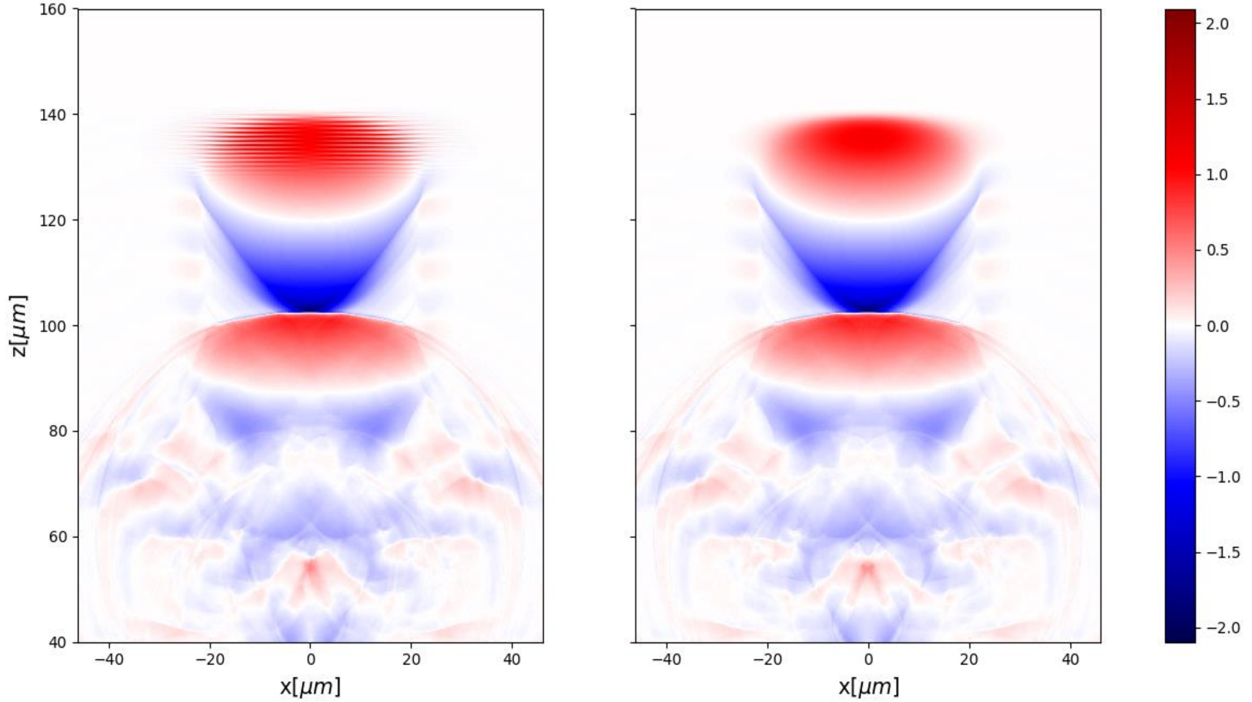
We simulated an ultra strong laser pulse that travels into a uniform electron plasma

$$a_0 = 15 \quad w_0 = 15\mu\text{m} \quad \tau_{fwhm} = 19\text{fs}$$

Density map (saturated)

PIC Envelope





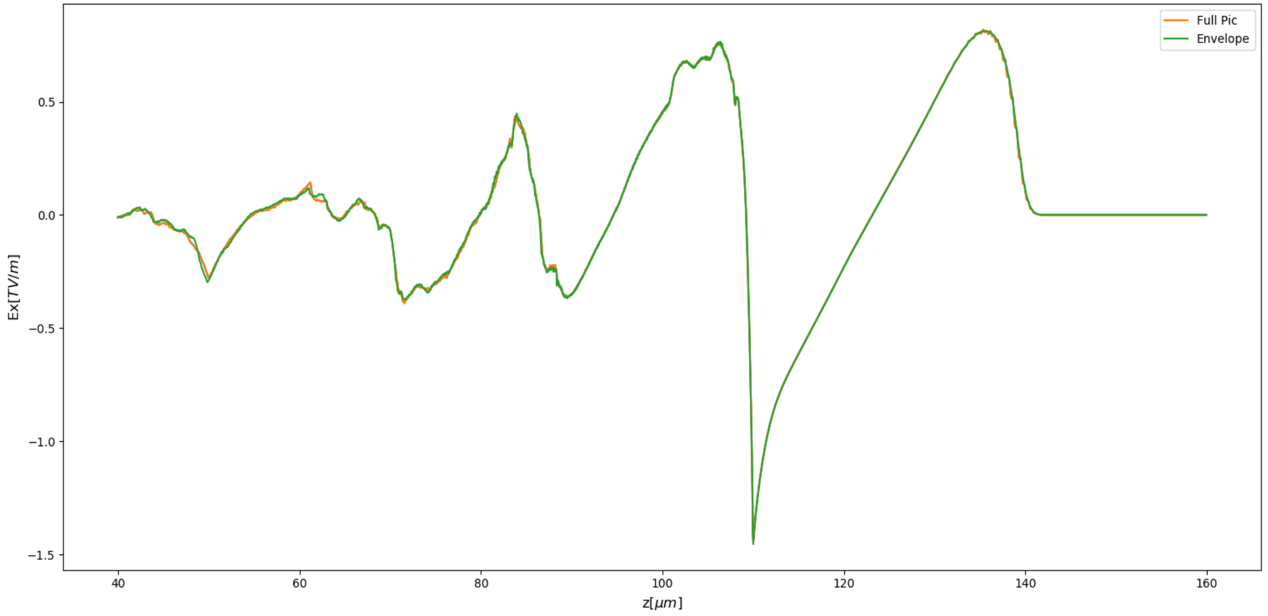
PIC Envelope

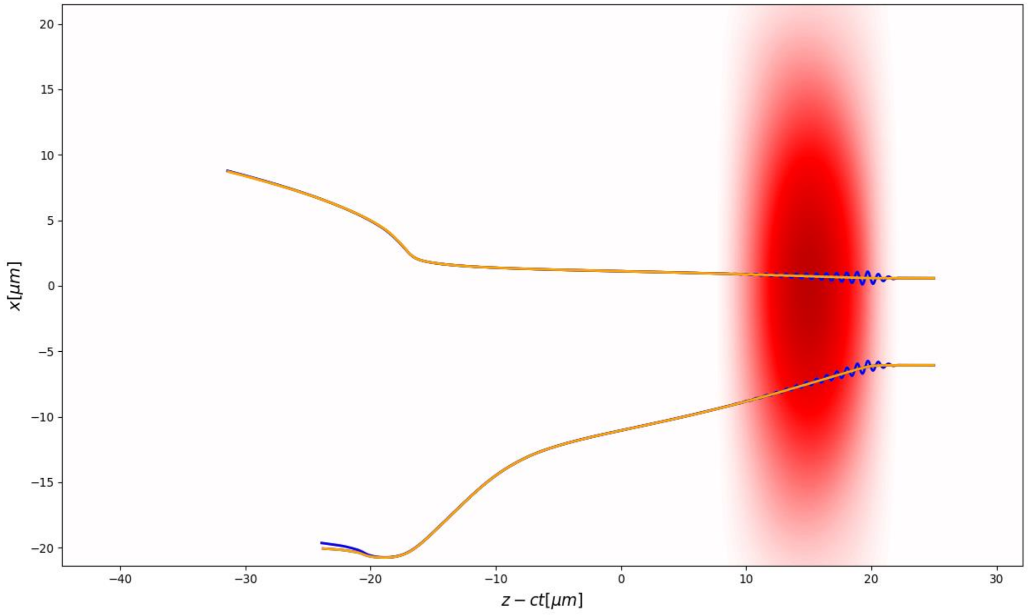
Longitudinal electric field

Benchmark against fully PIC simulations/2

$$a_0 = 15 \quad w_0 = 15\mu\text{m} \quad \tau_{fwhm} = 19\text{fs}$$

Longitudinal electric field lineout
(along propagation axis)





Tracked particle longitudinal momentum
in the fully PIC and Envelope scheme

Fluid approximation

Numerical resolution of the fluid equations in ALaDyn

$$\frac{1}{c}\frac{\partial}{\partial t}n + \nabla \cdot \left(\frac{\mathbf{u}}{\gamma} n \right) = 0$$

$$\frac{1}{c}\frac{d}{dt}\left(\mathbf{u} - \mathbf{a}\right) = -\frac{1}{2}\nabla\left(\frac{\mathbf{u}}{\gamma} \cdot \mathbf{a}\right) + \nabla\phi$$

Presents **several** nontrivial problems due to the advection and continuity equations → We converted the CFD literature to the case of the cold fluid plasma equations

WENO 3 + Adams-Bashfort discretization → We are able to evolve fields in the PIC framework

Hybrid PIC-Fluid

We developed and are constantly improving the possibility of evolving few macroparticles on a fluid background: **huge amount of computational time saved!**

Pro

- Don't need a lot of particles
- Less (a lot of!) memory usage
- Very fast

Cons

- Implementation not straightforward
- Cannot deal with strongly nonlinear dynamics

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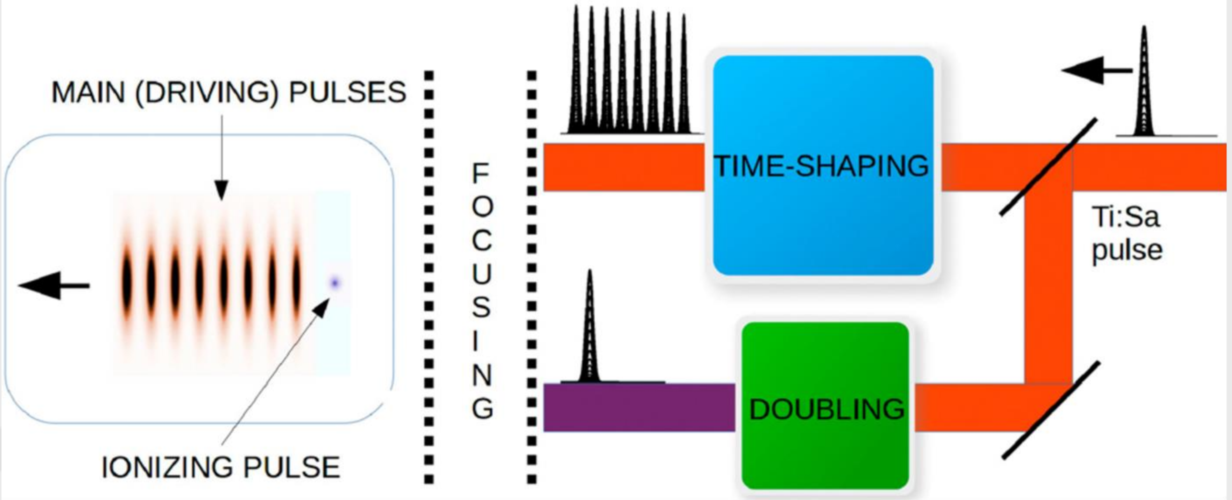
Innovative injection scheme

Experiments have shown accelerated bunches, but with a poor quality

New acceleration scheme proposed within the **EuPRAXIA** project

- Single 250-TW laser pulse
- Feasible with present technology
- Wakefield is excited by a train of pulses
- Particle bunch injected in the plasma ionizing a dopant with a frequency doubled (or tripled) pulse
- Beam emittance is kept low
- Experimental part is work in progress



European plasma research accelerator with excellence in applications

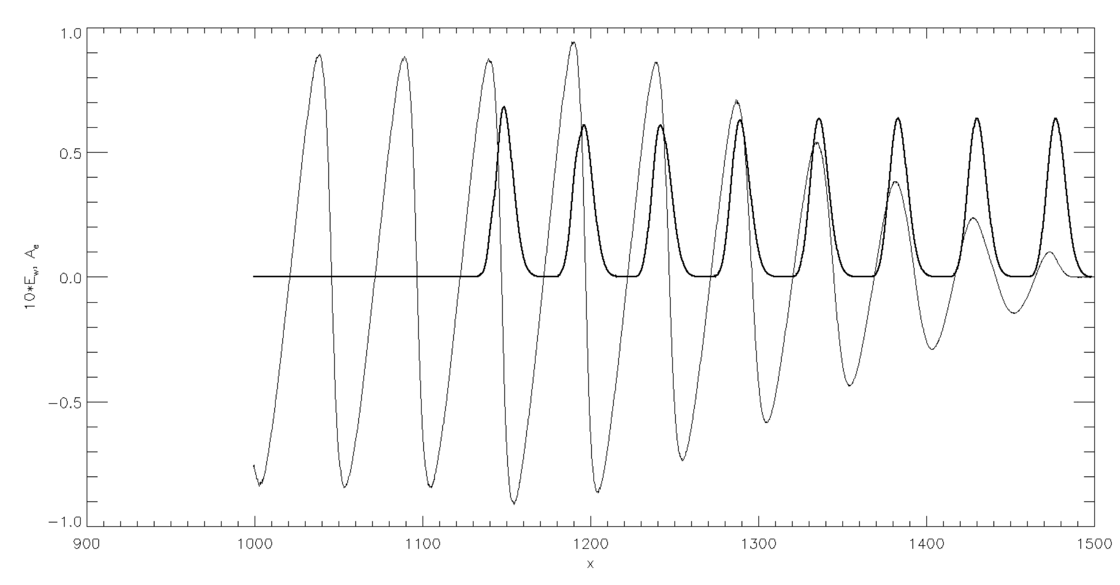
[Tomassini, De Nicola, Labate, Londrillo, Fedele, Terzani, Gizzi, *POP*, 2017 ,
Tomassini, De Nicola, Labate, Londrillo, Fedele, Terzani, Nguyen, Vantaggiato Gizzi, *NIMA*, 2018]

REsonant Multi-Pulse Ionization injection

To achieve better quality, wake generation and particle injection are separated

Wakefield

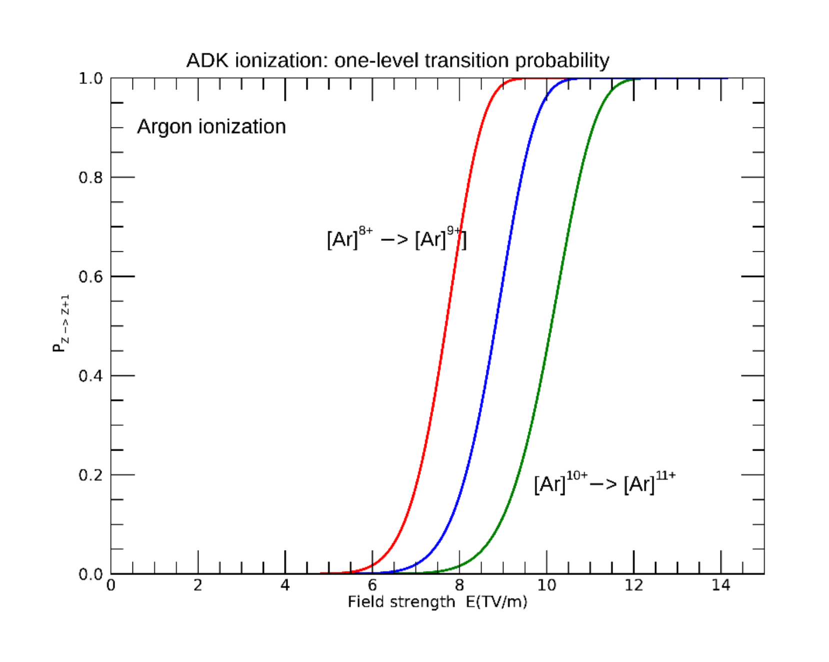
Main laser pulse is temporally reshaped as a train of pulses: **resonant process**



Wakefield more intense than with a single pulse

Electron bunch

ADK ionization to inject the electron bunch: tailoring of the bunch parameters



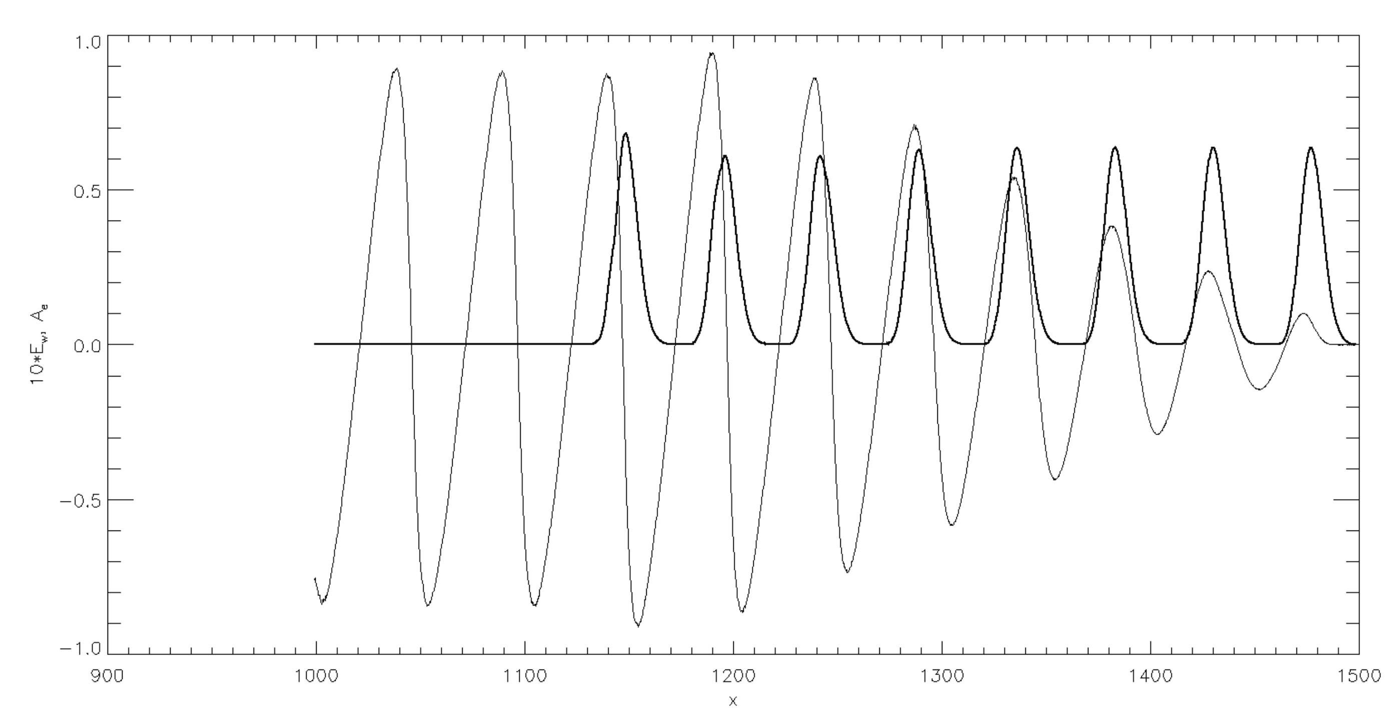
Wakefield generated by a train of pulses

A train of pulses of total energy E can generate larger wakefield respect to a single pulse of energy E

Divided the single excitation in a resonant process over many pulses

↓

Laser – plasma energy exchange is more efficient



Synchronize the forward and backward ponderomotive push of every pulse with the background density oscillations

Simulation of the REMPI scheme

- Eight laser driver to produce the wakefield
- One frequency doubled laser pulse to inject particles
- Very large pulse waist to avoid fast diffraction
- Independence of the system from the small frequencies

Largest and smallest length scales are very different and we only want to see the large motion

↓

Envelope approximation is very recommended

Strategy

Model design:

- Needs fast computational tool for a parameter scan
- Very reduced model: quasistatic approximation, plasma fluid description, 2D cylinidrical simmetry
- No consistent computational resource (laptop)

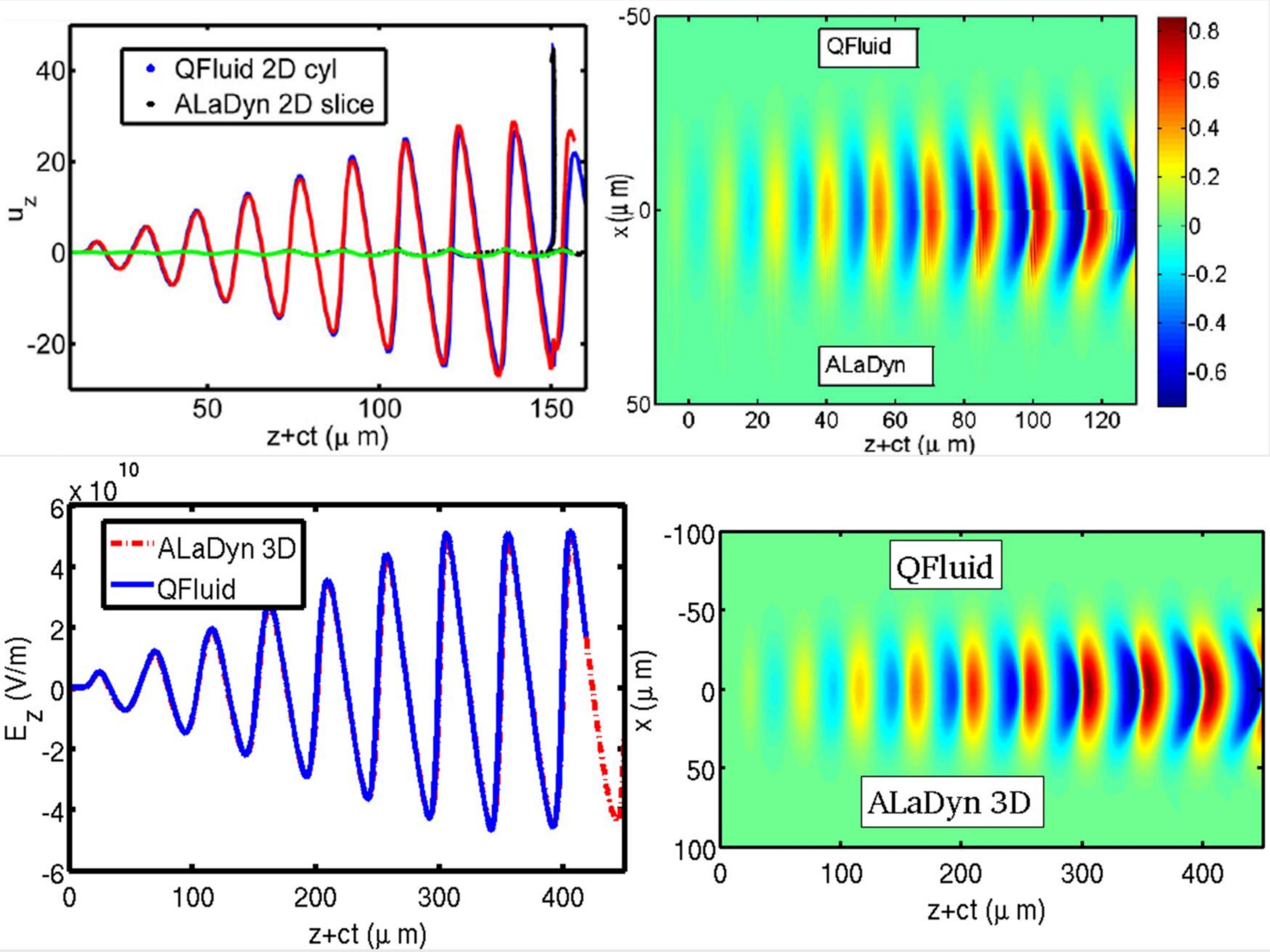
QFluid

Parameters finalization:

- Parameter space has already been reduced
- Fully selfconsistent (challenging) simulation
- Need computational resources from HPC (e.g. CINECA)

ALaDyn

First benchmark of the reduced simulations



2D test: Full physics

- Tested QFluid predictions in 2D
- Wakefield generation, atomic ionization and bunch formation
- Full PIC (Envelope was being developed)
- Quasistatic approximation holds (bunch formation is well predicted)

3D test: Wakefield dynamics

- Tested QFluid predictions in 3D
- Only wakefield generation is checked
- Full PIC (Envelope was being developed)
- QFluid and ALaDyn show the same fluid/kinetic motion

QFluid outcomes of the REMPI scheme

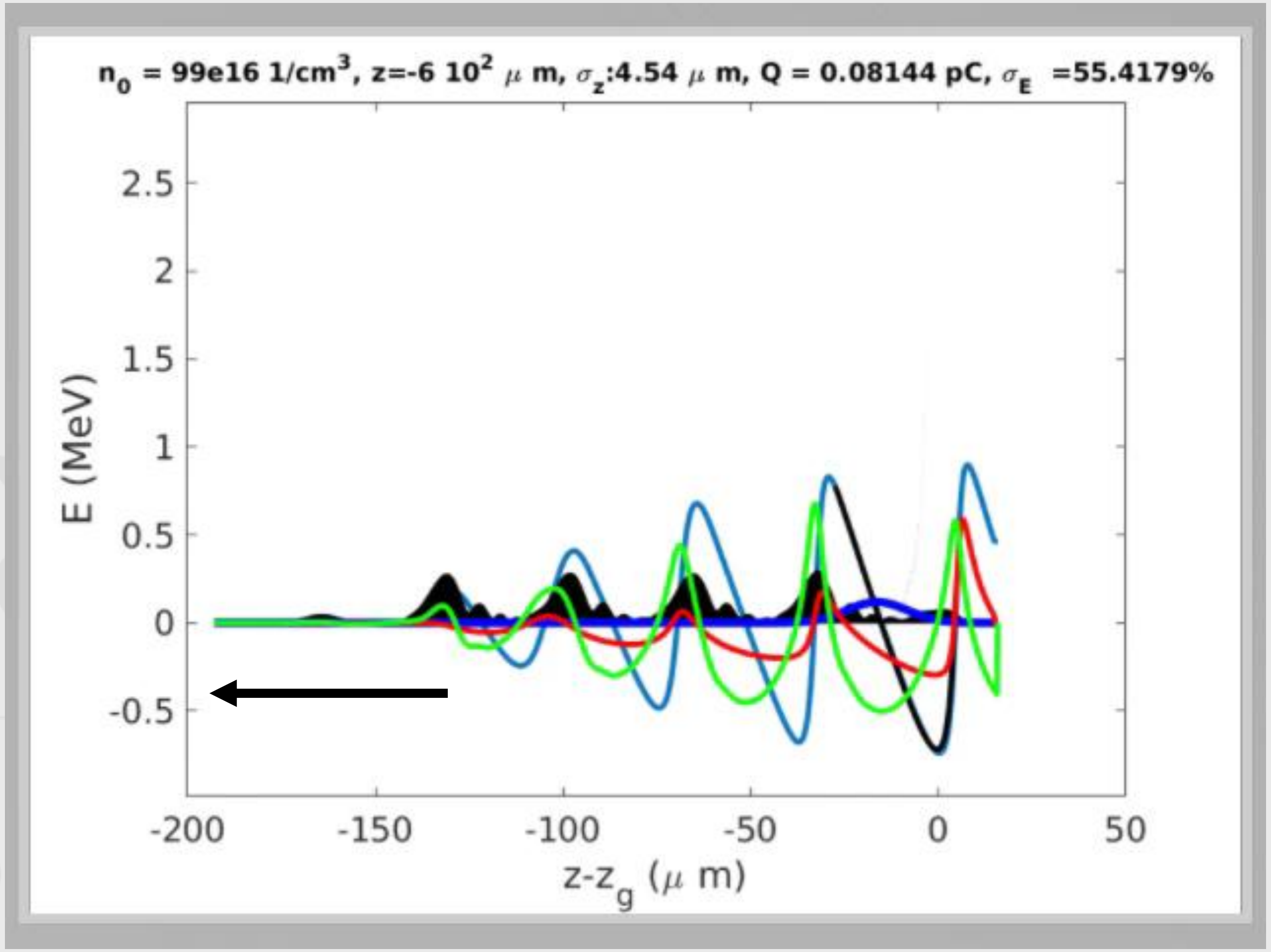
QFluid simulation:

- Evolving laser (Black, filled)
- Transverse electric field (Red)
- Longitudinal electric field (Blue)
- Radial force (Green)

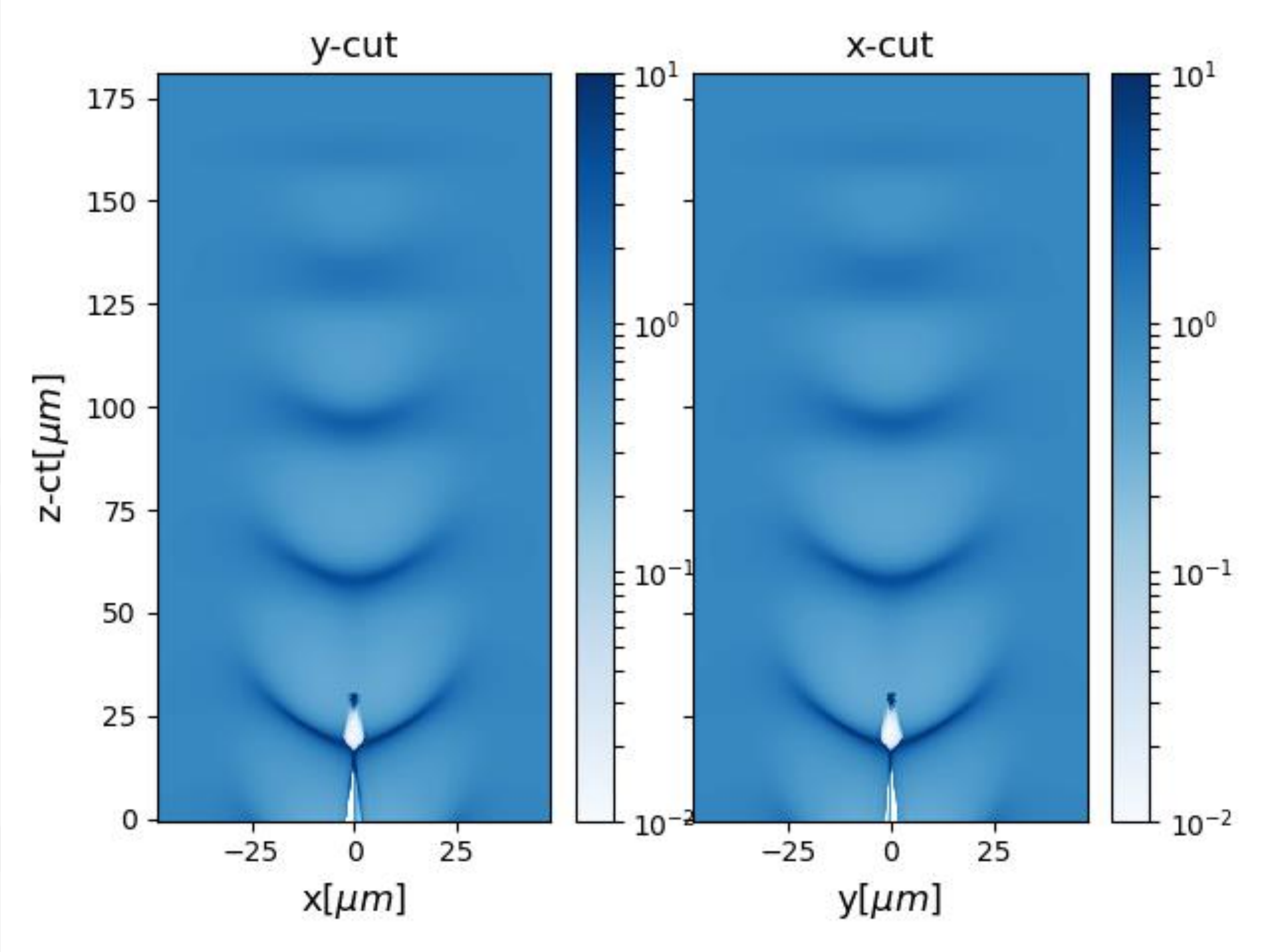
After 2 mm of propagation
Q=33 pC
E=140MeV,
ΔE/E=1.65%,

Double check with a full 3D PIC code is needed

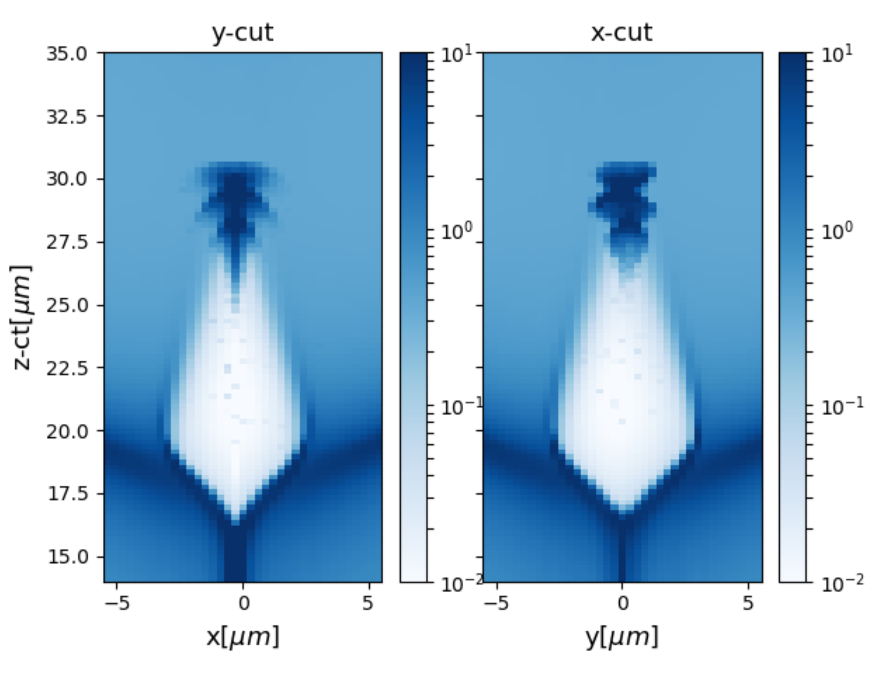
Courtesy of Paolo Tomassini, INO-CNR, Pisa



Comparison with ALaDyn



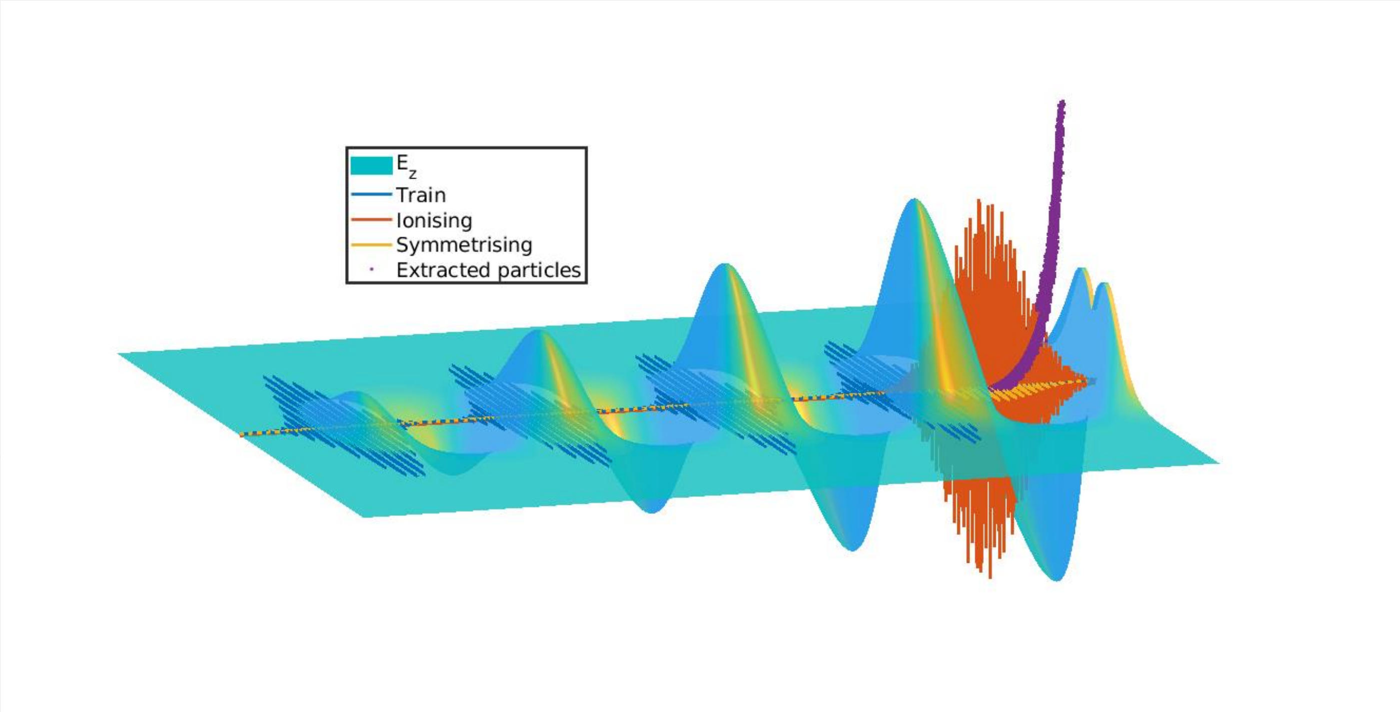
Density map + accelerated bunch obtained by ALaDyn in the first stage of REMPI configuration



Ongoning benchmarks

ALaDyn simulations are run with a fluid background + kinetic bunch particles in a 3D Cartesian geometry

- Bunch dynamics during charging (no quasistatic)
- Full 3D particle motion during acceleration (no axisymmetric)
- Plasma downramp to the plasma lens
- Off-axis stability tests (pointing jitter)



Conclusions

Challenging problems

- Produce high quality accelerated beams (low emittance and energy spread)
- Reduced models in plasma accelerator simulations are essential
- Envelope model relies on (common) physical requirement of the laser-plasma system
- Complete analytical theory is challenging, so, for extreme condition, it is an *a priori* assumption

Achievements

- We have developed a simple and fast algorithm for the envelope approximation that allows for a computational speed-up to orders of magnitude a standard PIC
- We applied ALaDyn's outcomes to benchmark an innovative injection and acceleration scheme for plasma acceleration
- REMPI would request a lot of computational resources to be simulated with a standard PIC, so the envelope model is a first step towards a start-to-end predictive simulation
- First results obtained by the REMPI scheme show an outstanding accelerated bunch quality, that could be applied for the coherent radiation generation in a X-FEL

Pisa, 14/03/2019

Thank you for your attention

Davide Terzani