Numerical implementation of a hybrid PIC-fluid framework in laser-envelope approximation

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Outline

1. ALaDyn: envelope and fluid solvers
   - Explicit envelope solver
   - Second order Envelope Boris pusher
   - Plasma equations in fluid approximation
2. High quality injection scheme
   - REMPI
   - Outcomes of the optimized injection scheme

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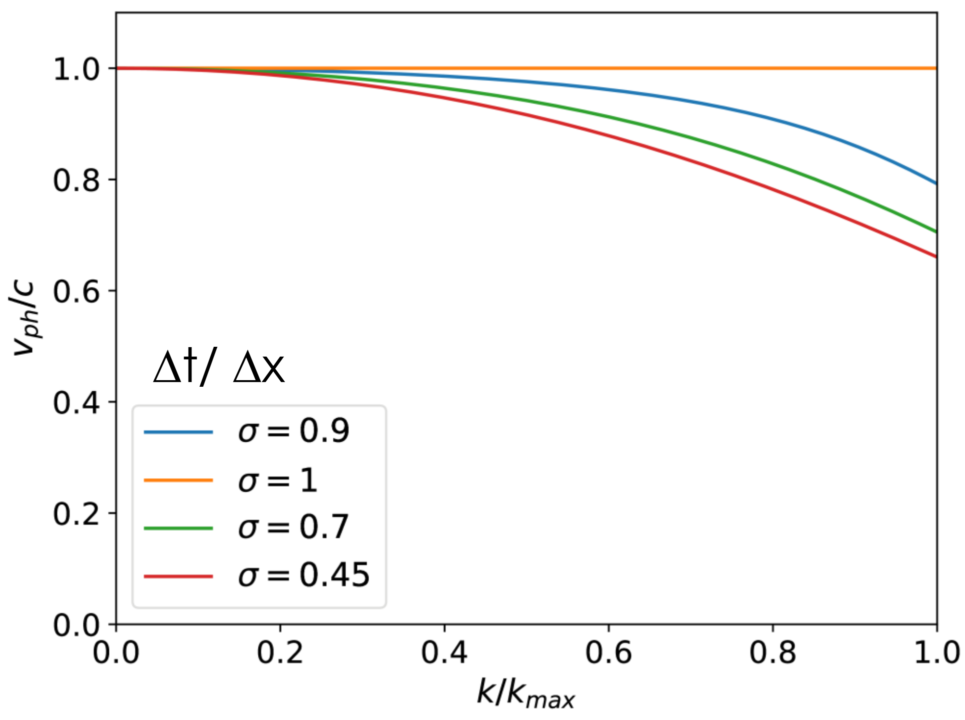
Particle-In-Cell limitations

Even though they are powerful, PIC codes present some limitations

- Numerical dispersion of electromagnetic waves
- High computational cost due to the number of particles
- Nonlinear 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

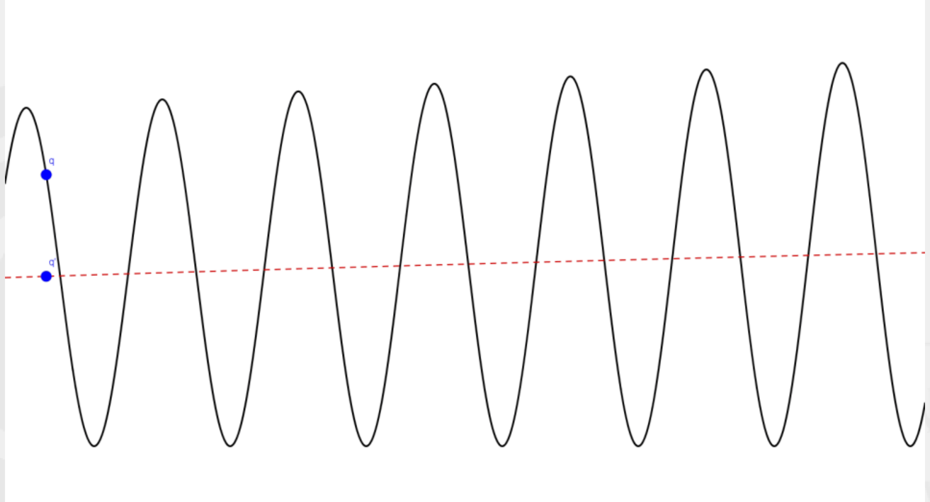
$$\lambda_0 \sim 1\mu\text{m},\ L_{tot} \sim 5\text{cm} \rightarrow T_{tot} \sim Mh$$

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

Multiscale expansion from a plane wave

Multiscale approximation starting from the **plane wave** solution

[Cowan, Bruhwiler et al., *JCP* 2011; Mora, Antonsen, *POP*, 1996]

Fast time scale $\sim \omega_0$

$\tilde{\mathbf{a}}_\perp(\xi),\ \tilde{\mathbf{u}}(\xi)$

Slow time scale $\sim \omega_p = \varepsilon \omega_0$

$\hat{\mathbf{a}}_\perp(\xi),\ \overline{\mathbf{u}}(\xi)$

$$\varepsilon = \frac{1}{k_0 w_0}$$

''Average'' motion: equations for slow varying components can be found if

$$\varepsilon \ll 1$$

$$1 - \frac{u_z}{\gamma} \gg \varepsilon$$

Time vatiations in a comoving r.f.

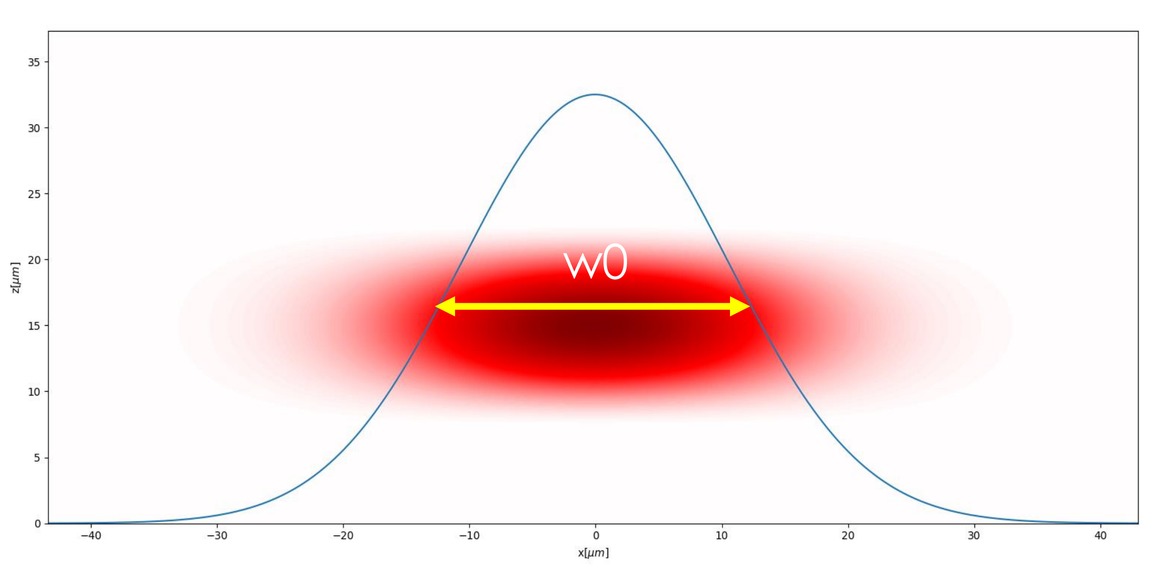
$$T_{Ray} = \frac{c\pi w_0^2}{\lambda_0} \qquad \partial_\tau \sim \mathcal{O}\left(\varepsilon^2\right)$$

Zeroth order results

$$\tilde{\mathbf{u}}_\perp = \tilde{\mathbf{a}}_\perp$$

$$\gamma - \beta u_z - \phi - 1 = 0$$

Lawson – Woodward theorem holds: no net energy gain



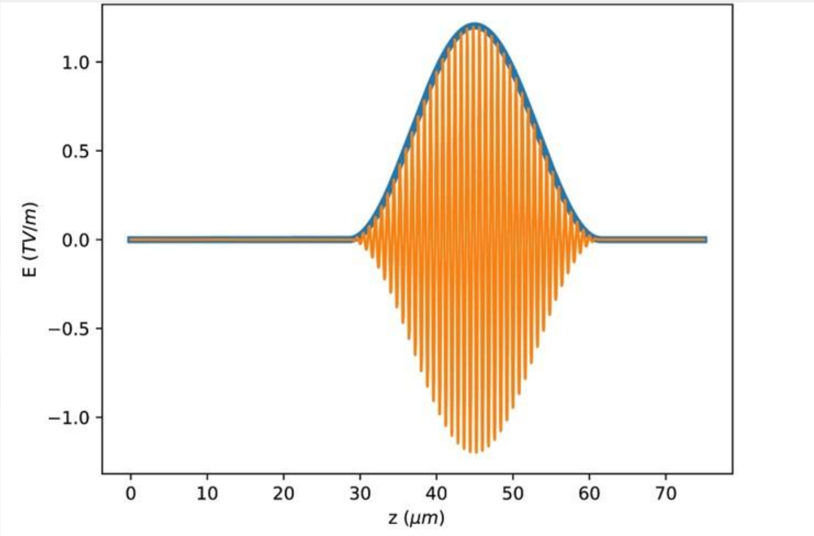
Laser envelope evolution equation

Maxwell's equation for vector potential

$$\left[\partial_{t,t} - 2i\omega_0(\partial_t + c\partial_z) - c^2\nabla^2\right]\mathbf{a}_\perp(\mathbf{x},t) + \cancel{c\nabla\partial_t\phi} = -\omega_p^2\mathbf{J}_\perp(\mathbf{x},t)$$

From Poisson's equation $\nabla\phi \sim \varepsilon\omega_0$

Laser pulse $\mathbf{a}_\perp(\mathbf{x},t) = \mathcal{R}e[\hat{\mathbf{a}}_\perp(\mathbf{x},t)e^{ik_0(z-ct)}]$



The average current can be written as

$$\widetilde{\mathbf{J}}_\perp = qn\frac{\widetilde{\mathbf{u}}_\perp}{\gamma} = \frac{\overline{n}}{\overline{\gamma}}\hat{\mathbf{a}}_\perp = \chi(\mathbf{x},t)\hat{\mathbf{a}}_\perp$$

We can express the slow varying factor as combination of slow varying quantities

$$\overline{\left(\frac{n}{\gamma}\right)} \simeq \frac{\overline{n}}{\overline{\gamma}}$$

[Mora, Antonsen, *POP*, 1996]

Comoving frame: No back propagating waves $(\xi = z - ct)$

$$\partial_{\tau,\tau}\hat{\mathbf{a}} - 2\left(i\omega_0 + \partial_\xi\right)\partial_\tau\hat{\mathbf{a}} - \nabla_\perp^2\hat{\mathbf{a}} = -\omega_p^2\chi\hat{\mathbf{a}}$$

Lab frame: fully selfconsistent equation

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

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

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

?

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**

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

Numerical evolution equation

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

Invert the formula by the means of centered derivatives

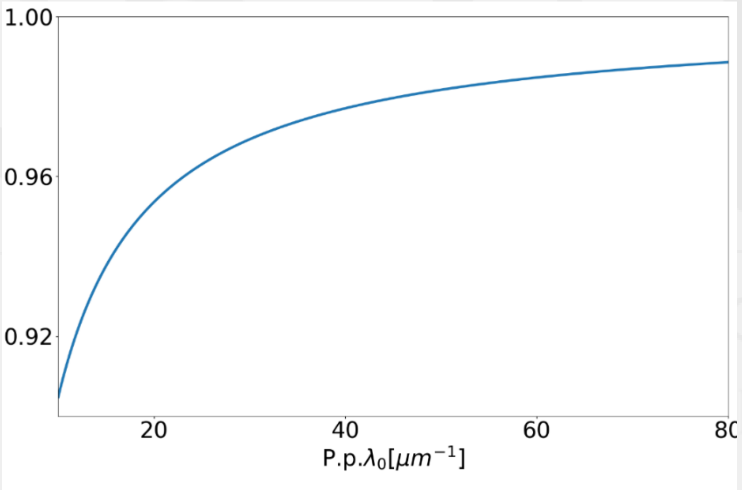
One step explicit advance

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

Stability

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

[Terzani, Londrillo, *CPC*, 2019]



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

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

Computing particles evolution

Revised version of the Boris pusher $\longrightarrow$ Recovers Boris pusher for no laser

Momentum update

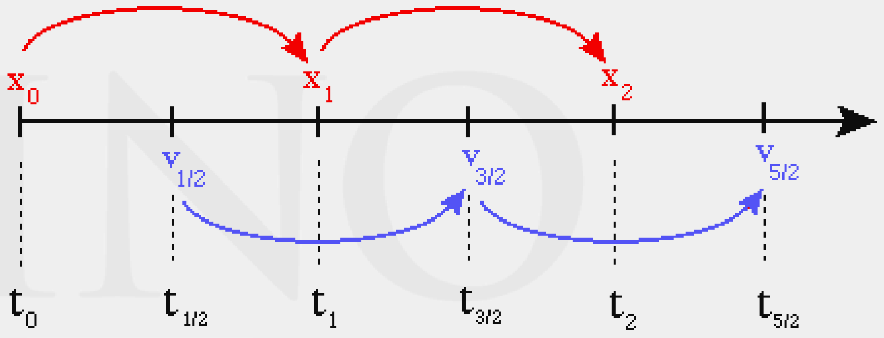
$$\boxed{u^n = \frac{1}{1+h^2}\left[w + w \times h + h(w \cdot h)\right]}$$

$$w = u^{n-1/2} + \frac{\Delta t}{2}\left(E^n - \frac{1}{4\widetilde{\gamma}_1}\nabla\left|a^n\right|^2\right)$$

$$h = \frac{\Delta t}{2\widetilde{\gamma}_1}B^n$$

Position update

$$\boxed{x^{n+1} = x^n + \Delta t\frac{u^{n+1/2}}{\widetilde{\gamma}_2}}$$



$\widetilde{\gamma}_1, \widetilde{\gamma}_2$ $\longrightarrow$ **Modified Lorentz factor** in the ponderomotive approximation $\longrightarrow$

$$\widetilde{\gamma}_1 = \left[\gamma_0^2 + 2\left(\widetilde{E} - \widetilde{a}/\widetilde{\gamma}_1\right)\cdot u^{n-1/2}\right]$$

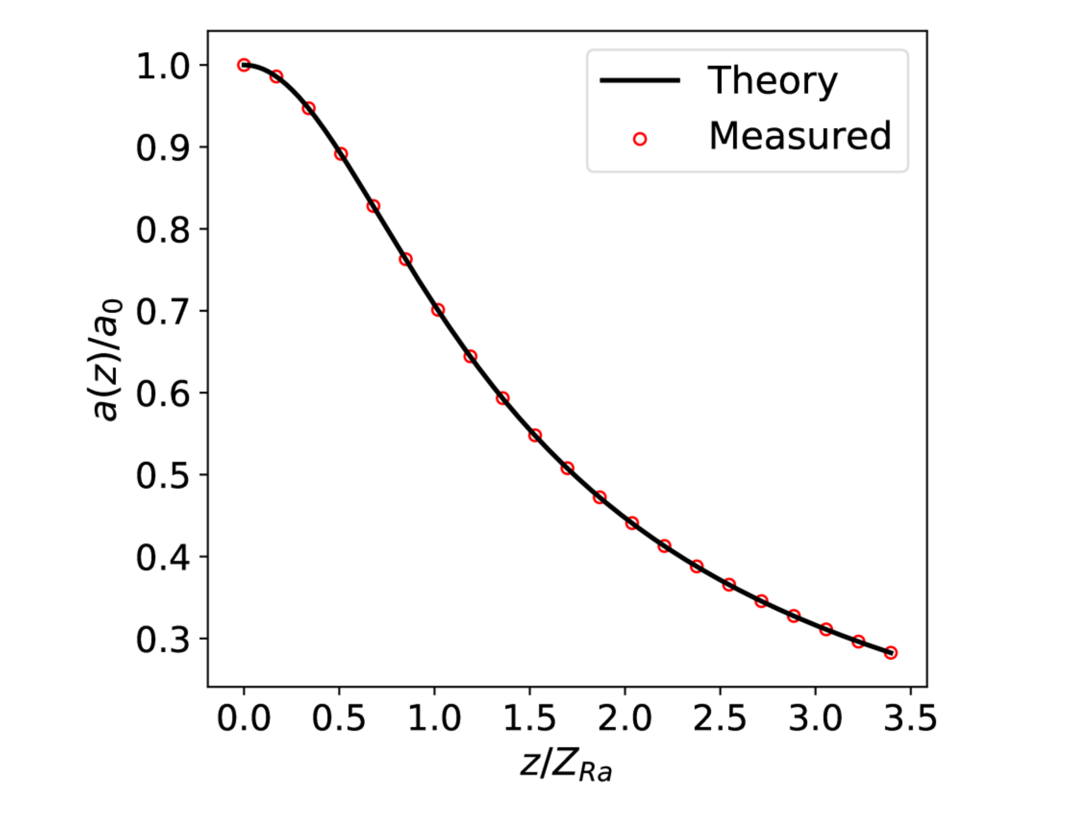
$$\widetilde{\gamma}_2 = \left[1/\gamma_0\left(1 - A\left(u \cdot \nabla|\widetilde{a}|^2\right)\right)\right]^{-1}$$

[Terzani, Londrillo, *CPC*, 2019]

Envelope benchmarks

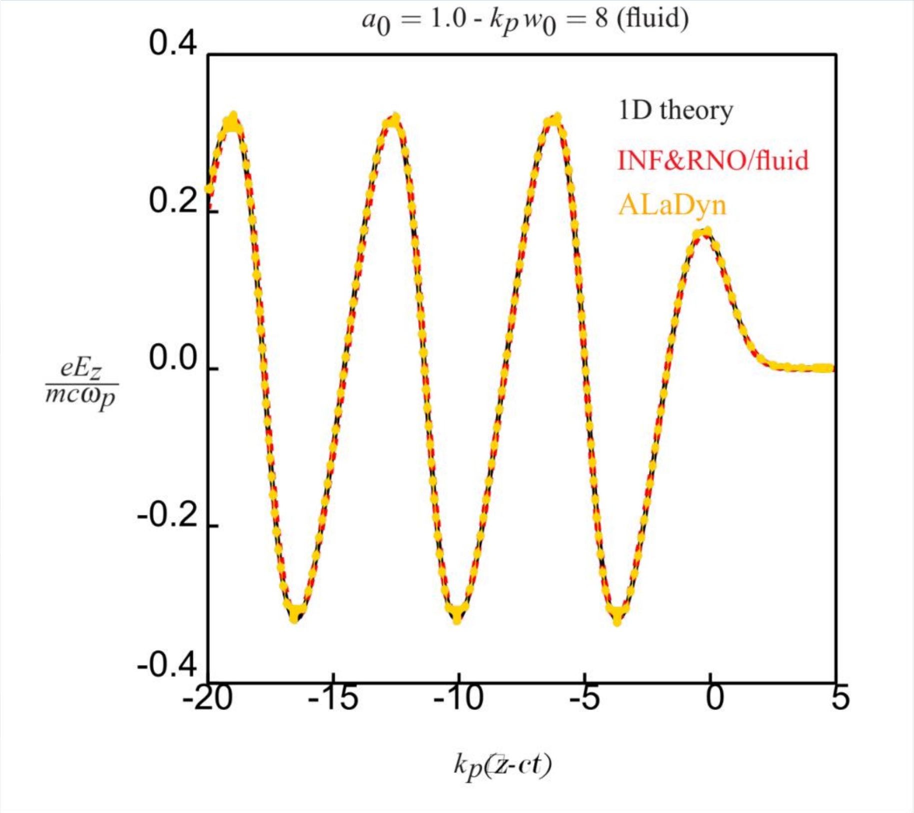
Rayleigh diffraction in vacuum

Verified correctness of laser solver



Longitudinal electric field in 1D approximation

Verified correctness of particle pusher



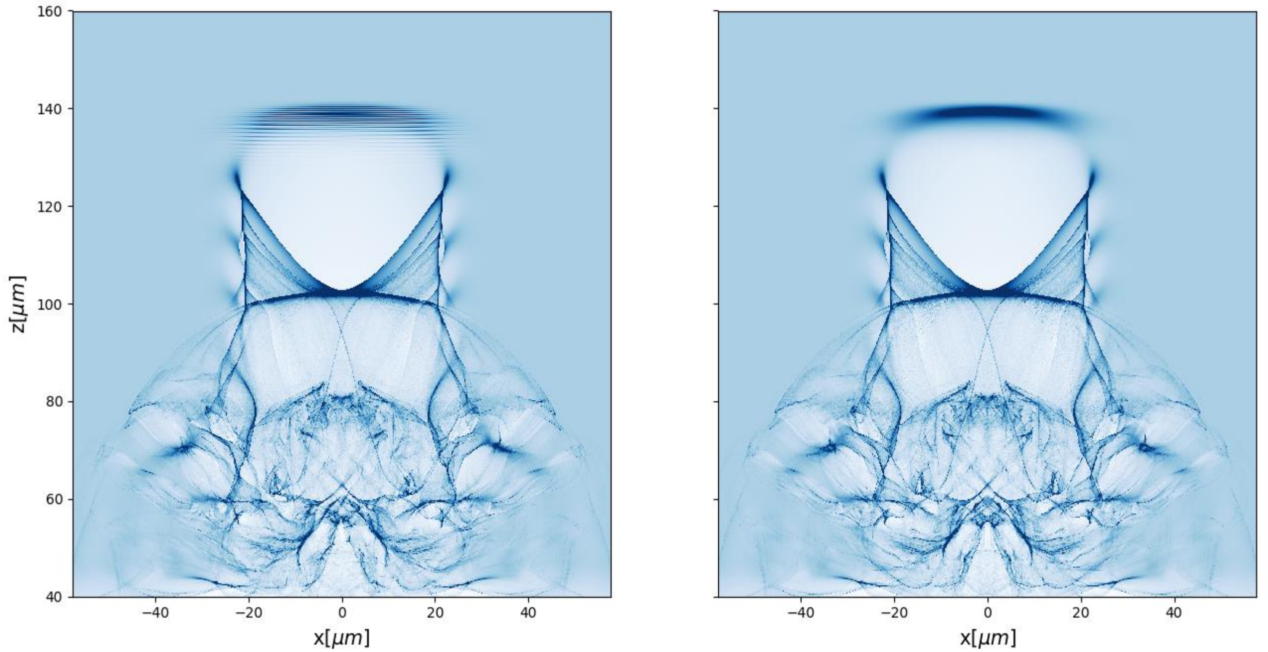
Envelope benchmarks/2

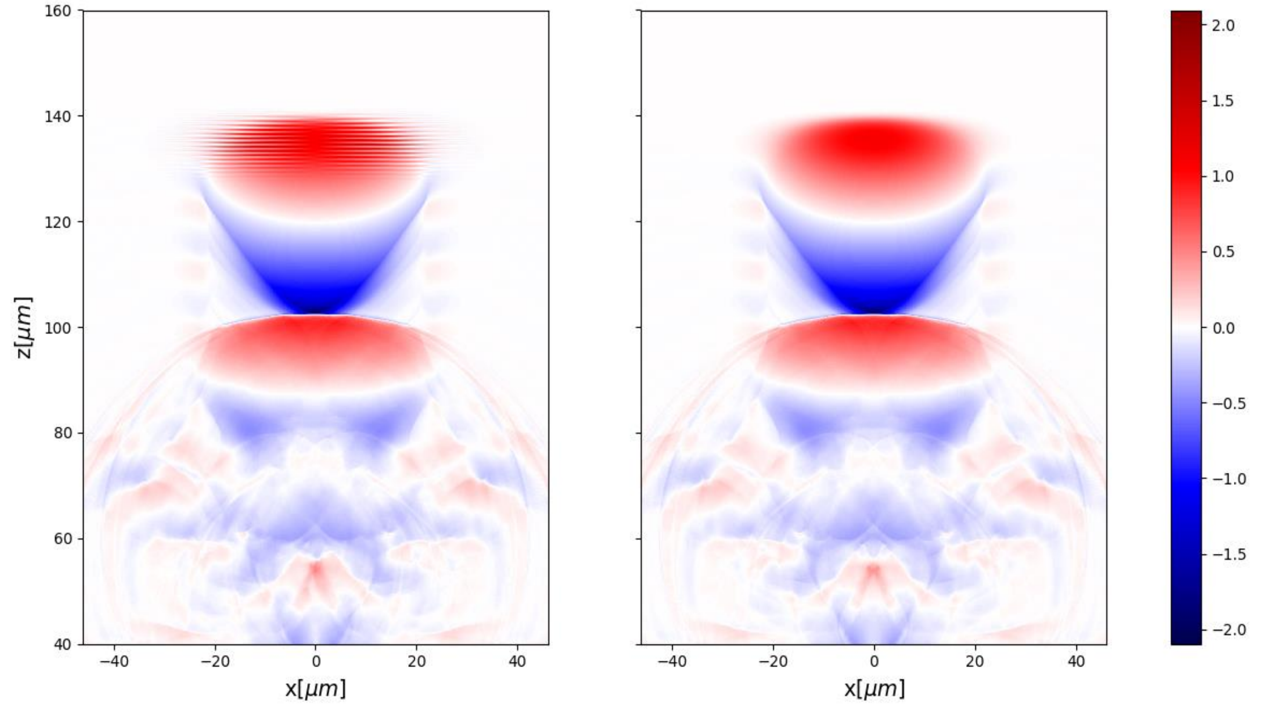
We simulated an ultra strong laser pulse that travels into a uniform electron plasma

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

Density map (saturated)

PIC Envelope





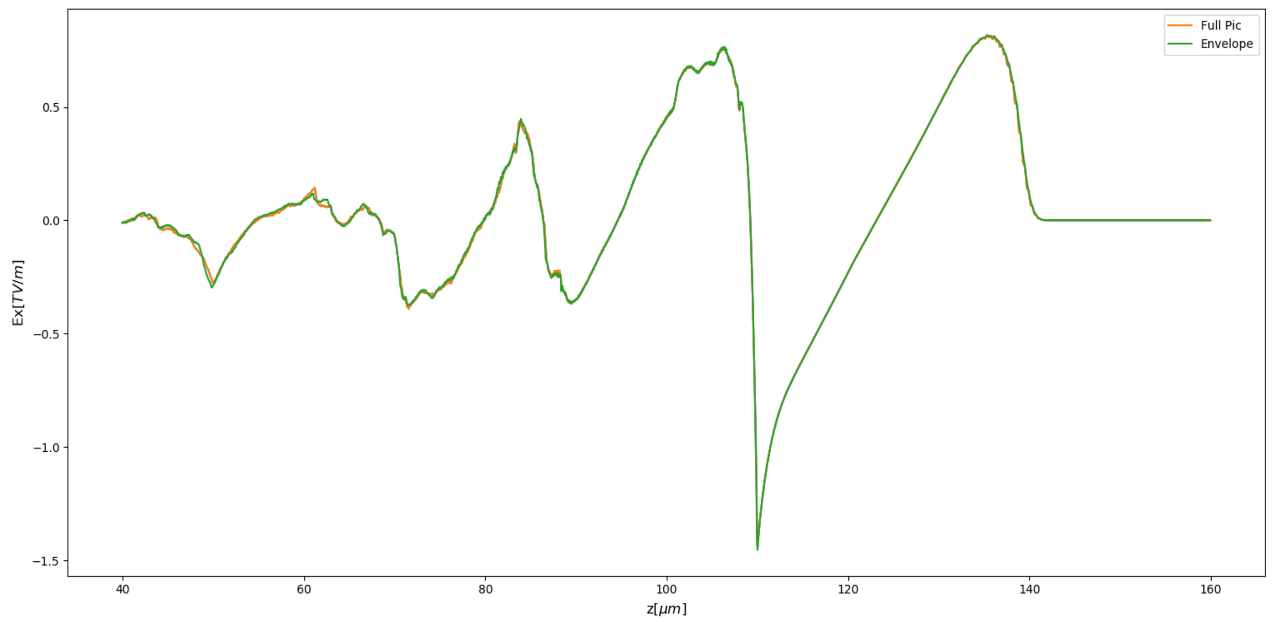
PIC Envelope

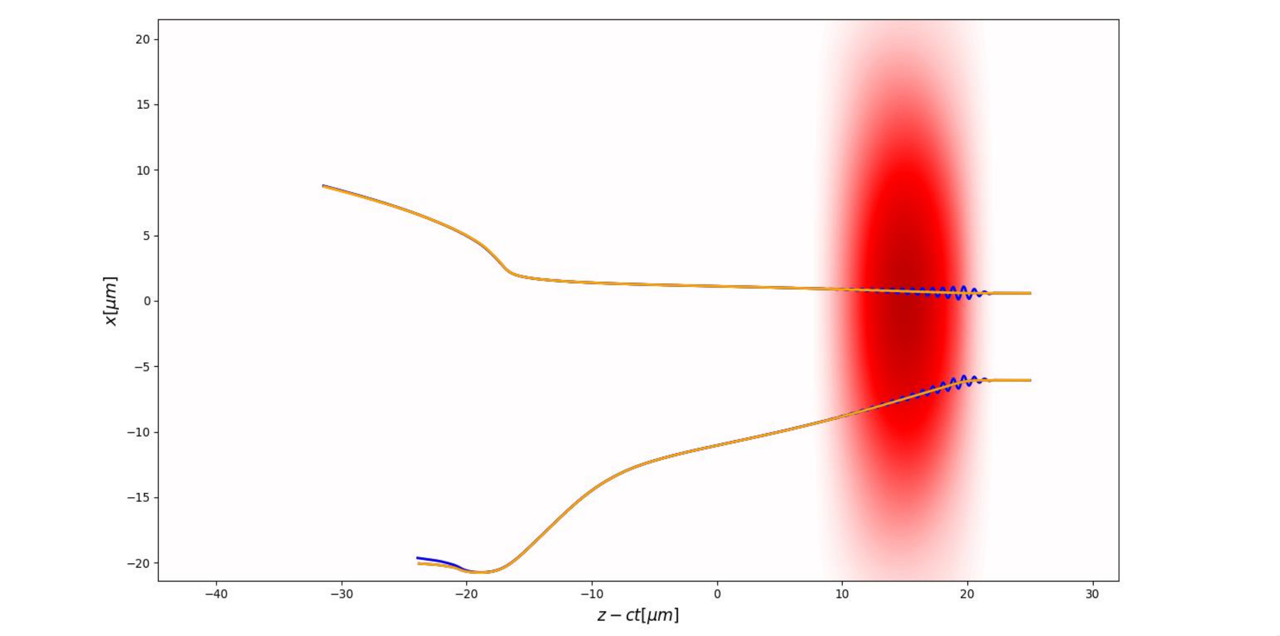
Longitudinal electric field

Envelope benchmarks/3

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

Longitudinal electric field lineout (along propagation axis)





Tracked particle longitudinal momentum in the fully PIC and Envelope scheme

Cold fluid approximation

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

$$\frac{1}{c}\frac{\partial}{\partial t}\mathbf{u} + \left(\frac{\mathbf{u}}{\gamma}\cdot\nabla\right)\mathbf{u} = q\left(\mathbf{E} + \frac{\mathbf{u}}{\gamma}\times\mathbf{B}\right)$$

$(n,\, \mathbf{u})$

Averaged on momentum space → Plasma is described making use of 3D (spatial) functions

In case of ponderomotive approxiamtion

Valid until kinetic effects arise: **density and momentum must be single – valued**

$$\gamma \rightarrow \gamma_P$$

$$q\left(\mathbf{E} + \frac{\mathbf{u}}{\gamma}\times\mathbf{B}\right) \rightarrow q\left(\mathbf{E}_w + \frac{\mathbf{u}}{\gamma}\times\mathbf{B}_w\right) + \mathbf{F}_P$$

Pros
- Doesn’t need a lot of particles
- Less (a lot of!) memory usage
- **Very fast**

Cons
- Implementation not straightforward
- Loses accuracy near the **wavebreaking**

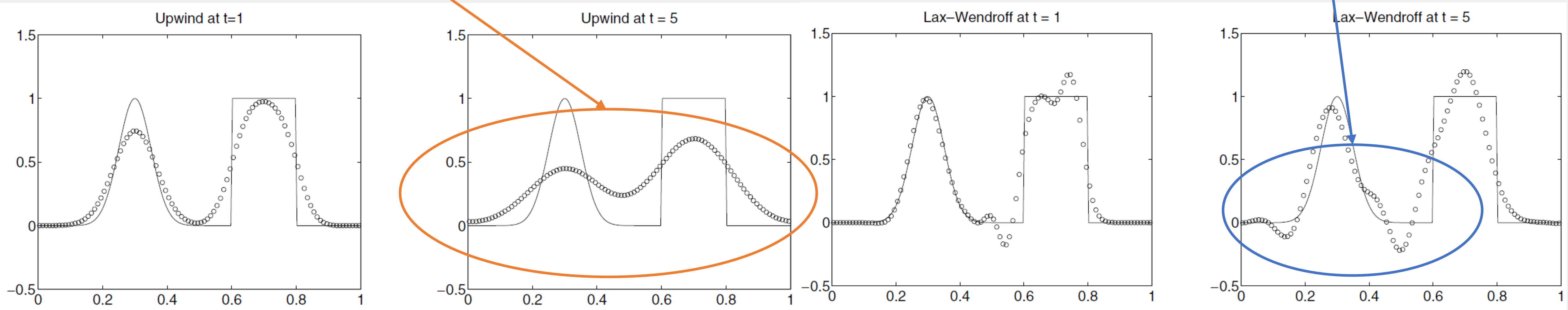
Computational Fluid Dynamics

Several nontrivial problems related to the hyperbolic structure of the equations.

Numerical induced **dissipation**

Do not preserve **positivity** (density)

Unstable **oscillations**



Even for linear hyperbolic equations

[Leveque, *Finte volume methods for hyperbolic equations*]

Implementation in ALaDyn

Huge literature available for hyperbolic equations for conservative and compressible Euler equations

→

Plasma (relativistic pressureless Euler + Maxwell's equations)

Easier in non – conservative form

No natural diffusive term

[Terzani, Londrillo, *CPC*, 2019]

Consistent with **ALaDyn's framework**

- Second order Boris pusher for particle dynamics
- Electromagnetic field solved on a staggered spatiotemporal grid (FDTD)

Particle and fluid dynamics can cooperate for a hybrid approach

$$\partial_t \mathbf{u} = \mathbf{L}\left[\mathbf{u}, \mathbf{x}, t\right]$$

Adams-Bashfort discretization

$$\mathbf{L}\left[\mathbf{u}, \mathbf{x}, t\right] = \mathbf{F}_L - \left(\frac{\mathbf{u}}{\gamma} \cdot \nabla\right) \mathbf{u}$$

Weighted Essentially Non – Oscillatory Reconstruction (**WENO**)

Temporal integration

Adams – Bashfort method

$$\mathcal{D}_t\mathbf{u} \simeq \partial_t\mathbf{u} + c_1\Delta t^2\left[\frac{\partial^3\mathbf{u}}{\partial t^3}\right] + c_2\Delta t^3\left[\frac{\partial^4\mathbf{u}}{\partial t^4}\right]$$

- Method is one step (faster)
- Second order accuracy
- Consistent with PIC Electromagnetic and particle solver

Leading order **dispersive** plus a small **dissipative** error

$$\partial_t\mathbf{u} = \mathbf{F}\left[\mathbf{u},\mathbf{x},t\right] \qquad \mathbf{u}^{n+1} = \mathbf{u}^n + \frac{3}{2}\Delta t F^n - \frac{1}{2}\Delta t F^{n-1}$$

Source term known at integer times: compatible with Maxwell solver

Spatial integration

2^{nd} **order WENO** reconstruction

$$\mathbf{S_u}\left[\mathbf{u},\mathbf{x},t\right] = \mathbf{F}_L - \left(\frac{\mathbf{u}}{\gamma}\cdot\nabla\right)\mathbf{u}$$

$$\mathbf{S}_n\left[\mathbf{u},\mathbf{x},t\right] = -\nabla\cdot\left(\frac{\mathbf{u}}{\gamma}n\right)$$

Reconstruct $\frac{u}{\gamma}, u$ and n values using grid (known) points such that (1D example)

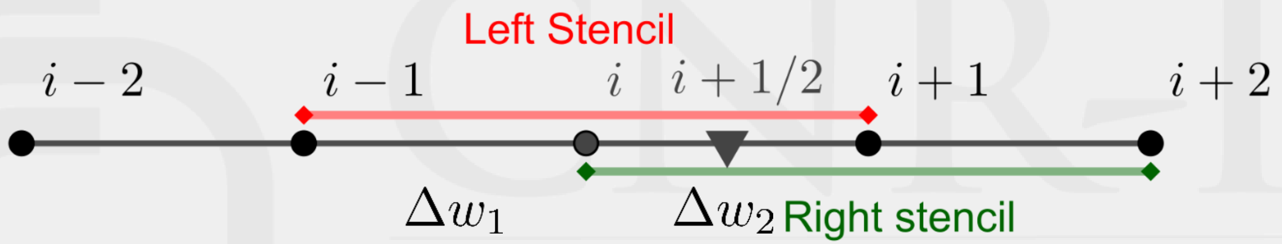
$$\frac{\widehat{w}_{i+1/2} - \widehat{w}_{i-1/2}}{\Delta x} = \partial_x w + \mathcal{O}\left(\Delta x^3\right)$$

Could be of any order

Choice of the interpolating stencil

$$\widehat{w}^L_{i+1/2} = w_i + \frac{1}{2}\left(c_1\Delta w_1 + c_2\Delta w_2\right)$$

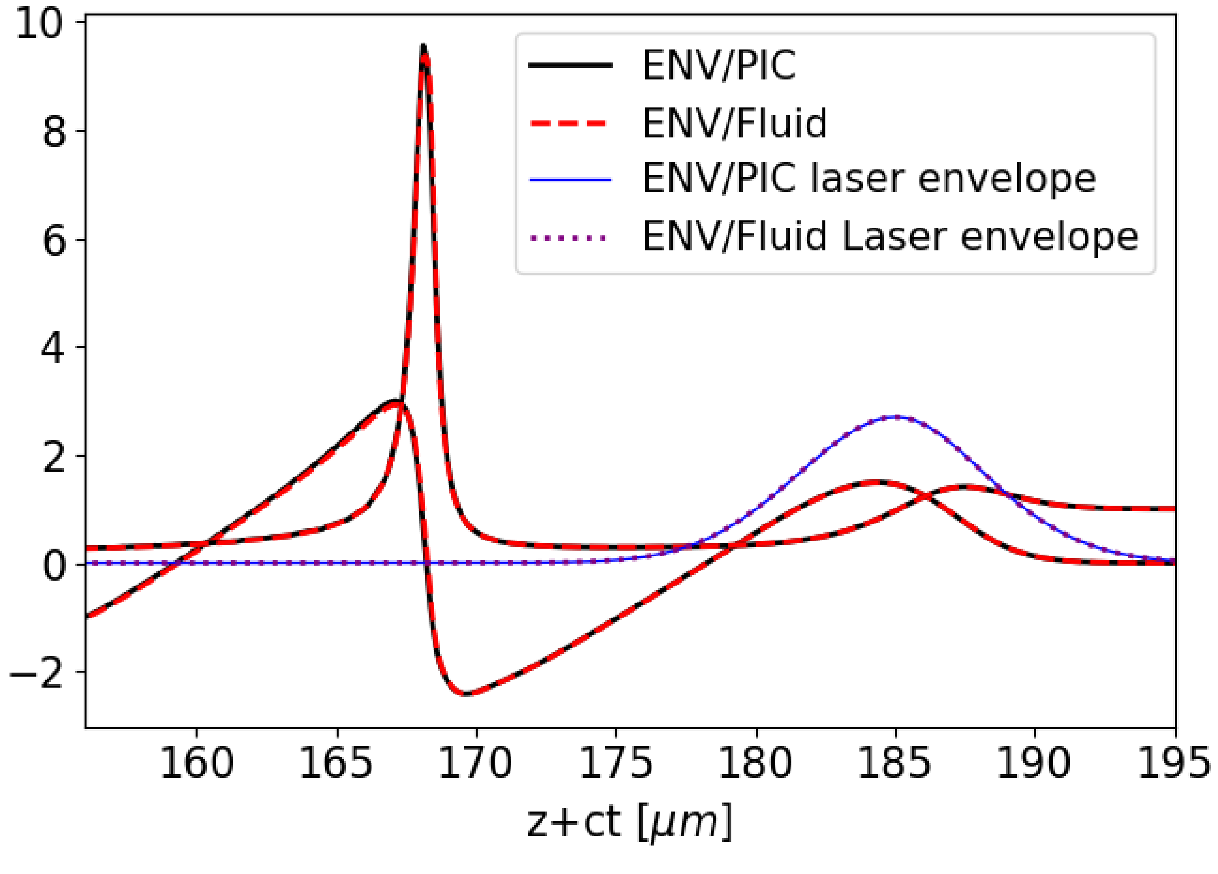
$$\widehat{w}^R_{i-1/2} = w_i - \frac{1}{2}\left(c_2\Delta w_1 + c_1\Delta w_2\right)$$

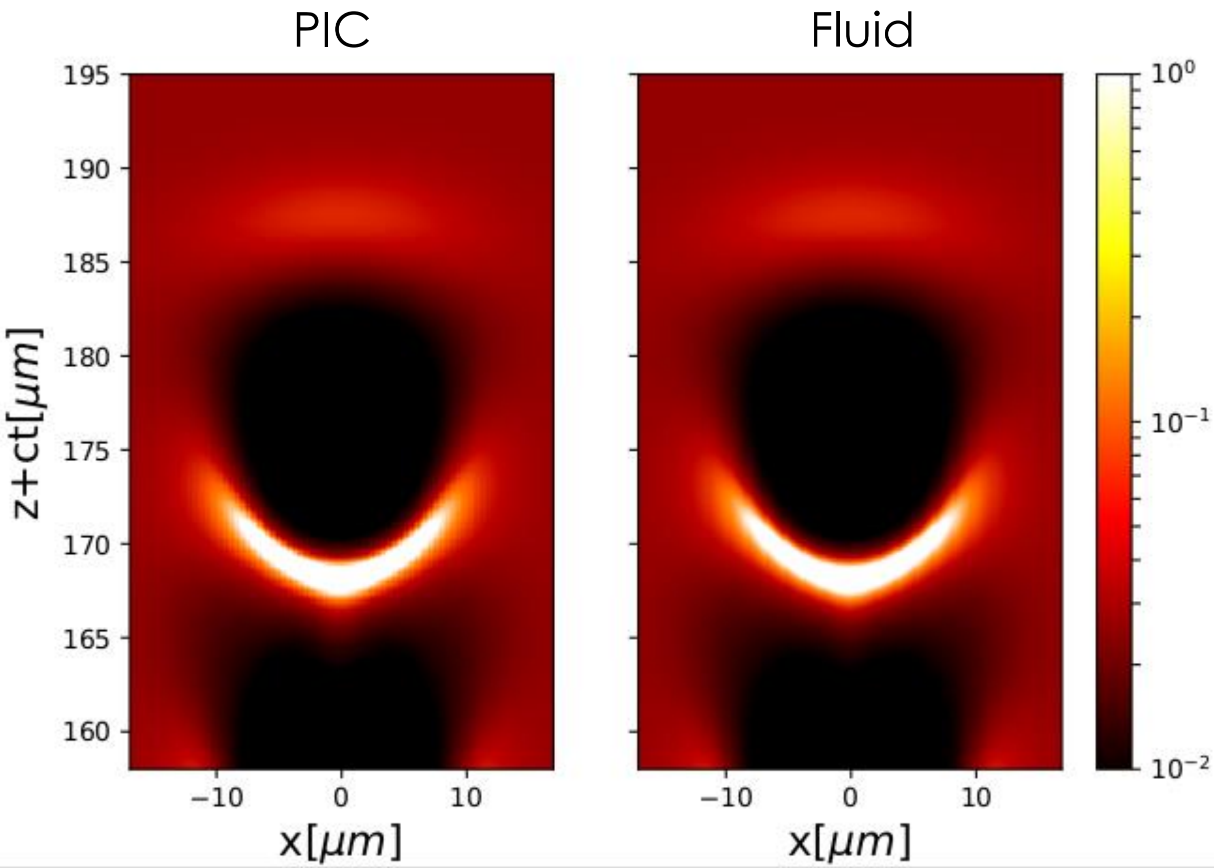


In WENO scheme c_1 and c_2 are nonlinear weights to assure **smoothest non oscillatory solution**

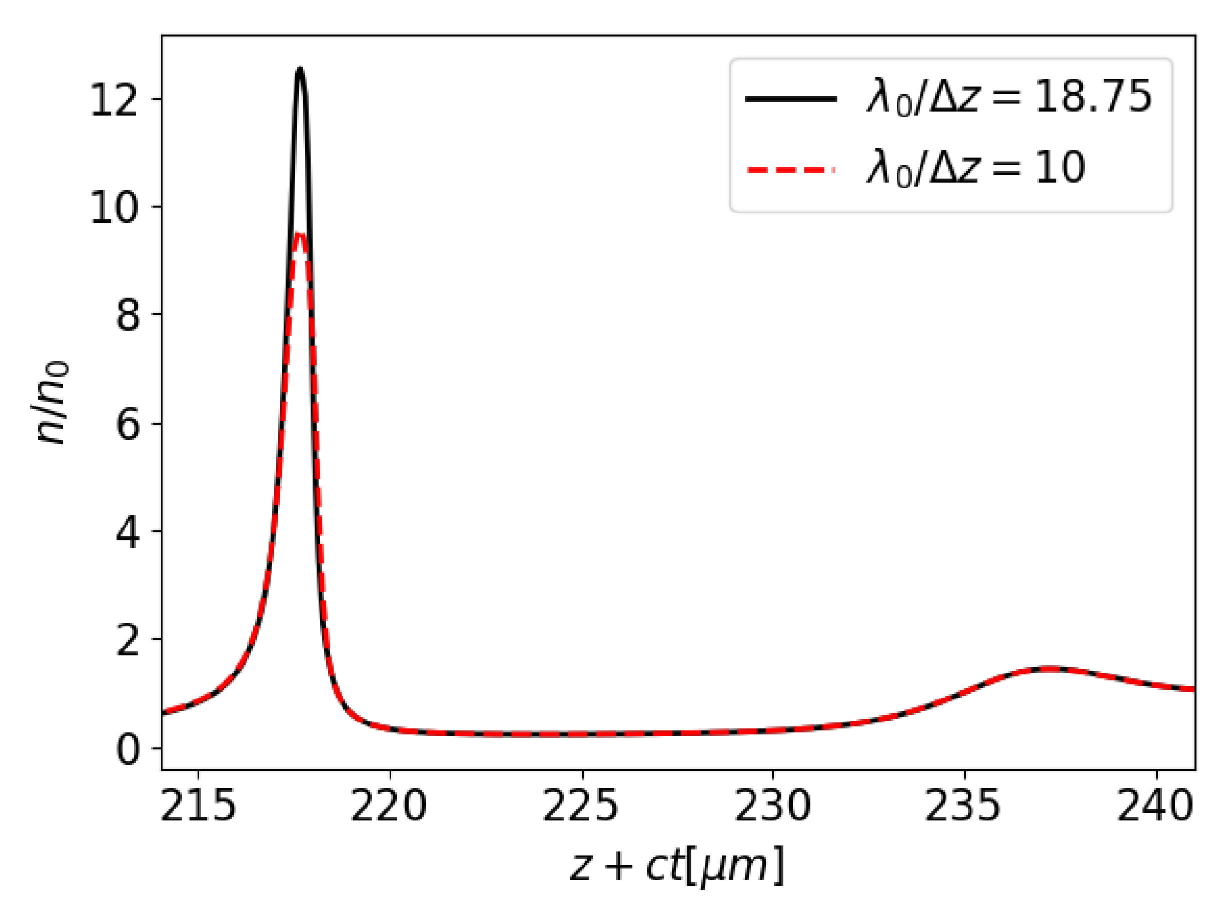
Eulerian integrator benchmarks

$$a_0 = 2.5 \quad w_0 = 12.7\,\mu\text{m} \quad \tau_{fwhm} = 20\,\text{fs} \quad n_0 = 4.25 \times 10^{18}\text{cm}^{-3} \quad \lambda_0/\Delta z = 18.75$$





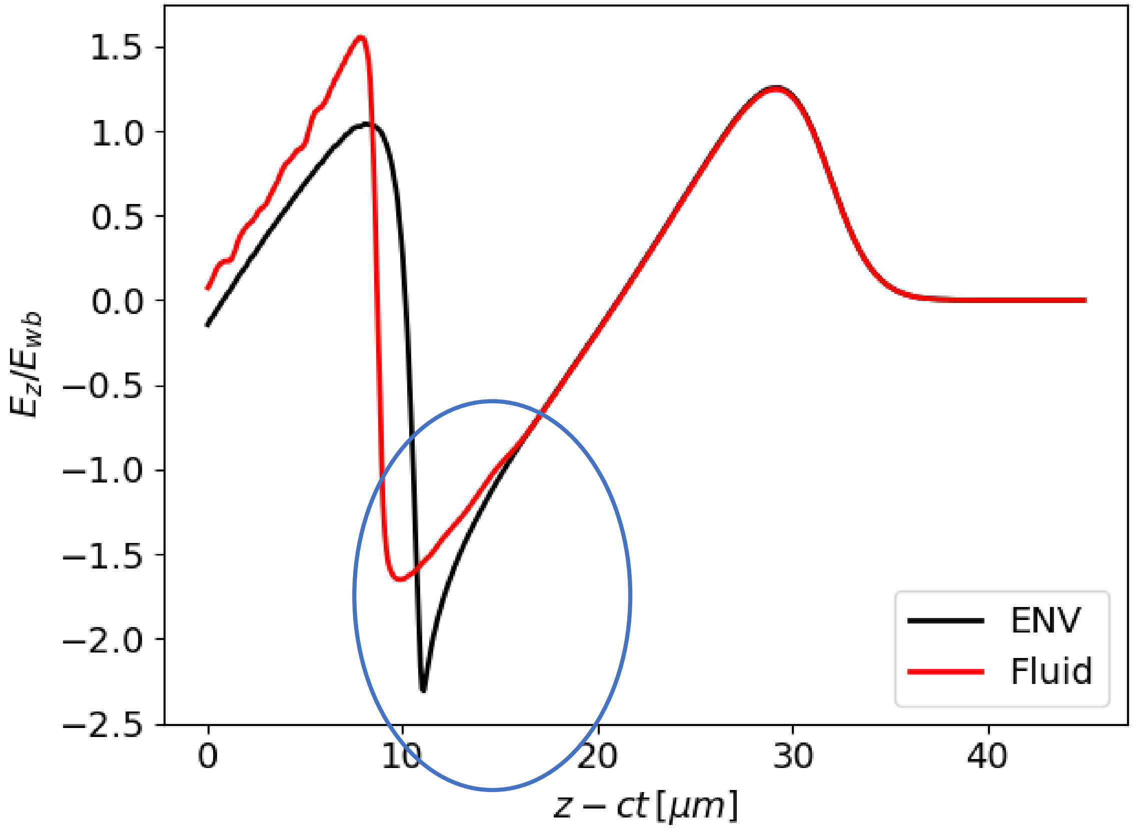
Eulerian integrator benchmarks/2

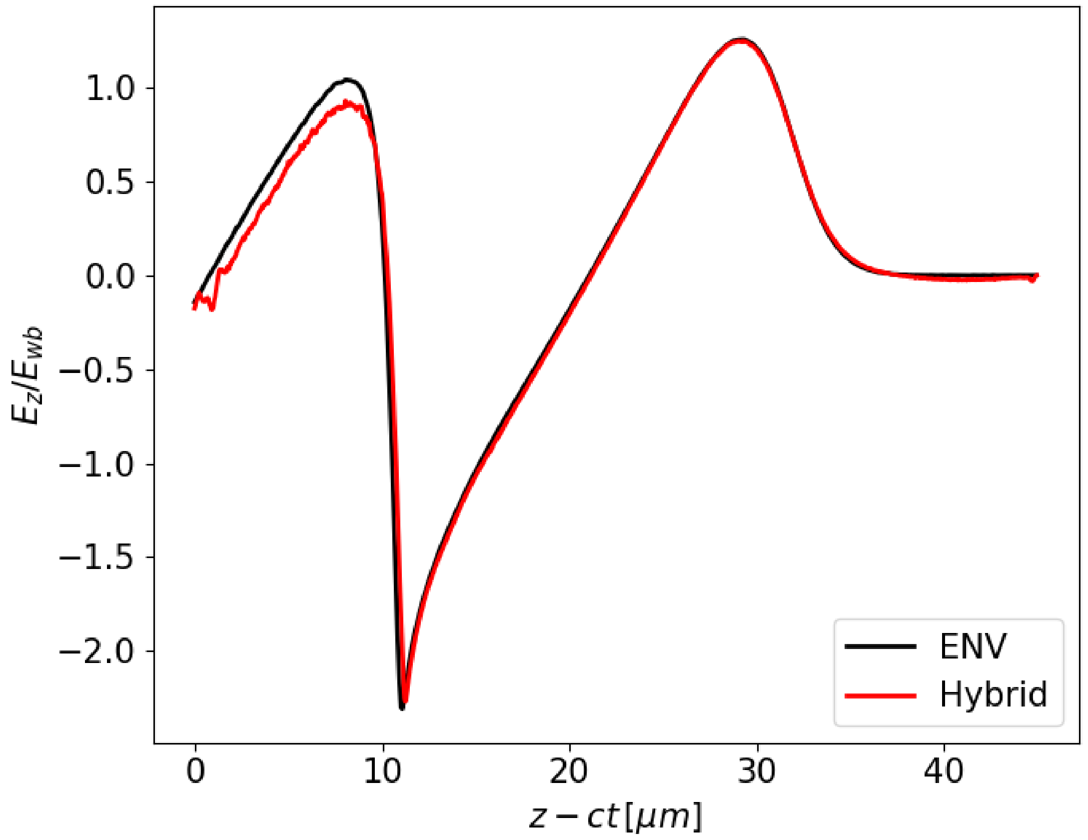


For lower resolution, **numerical dissipation** is very strong

Can higher order temporal and spatial schemes reduce the numerical dissipation and allow to simulate stronger nonlinearities?

Towards strongly nonlinear regimes (preliminary)





Fluid theory is reaching the limit of validity → Let us add some particles

Numerically the discontinuity is smeared

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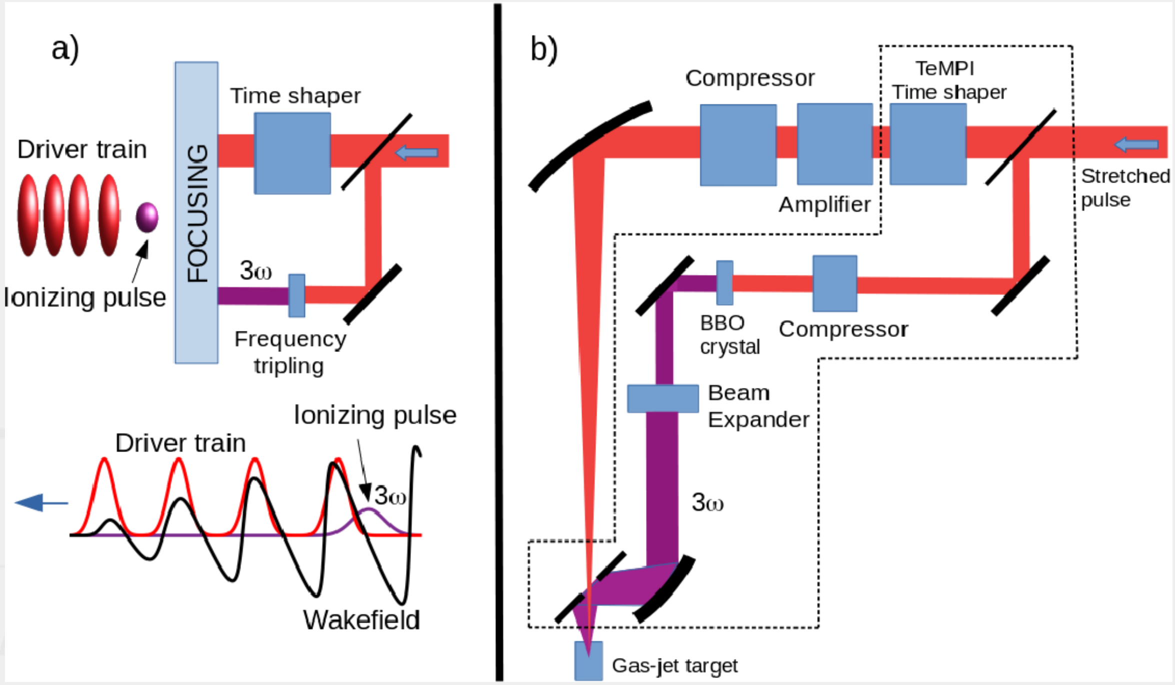
High quality injection scheme

Experiments have shown accelerated bunches, but with a poor quality

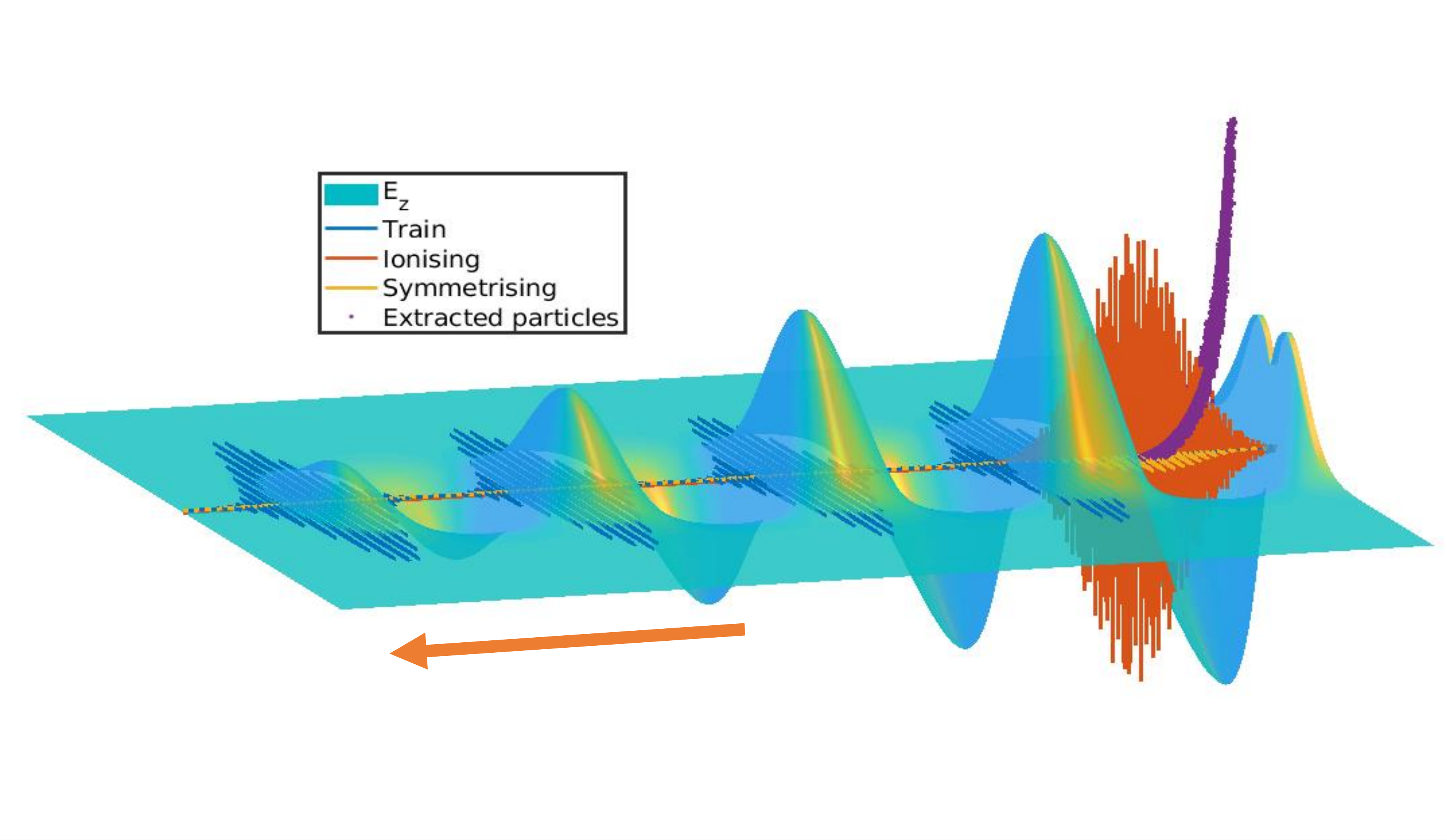
New acceleration scheme proposed within the **EuPRAXIA** project

- Single 150 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 realization is WIP



[Tomassini *et al., POP*, 2017
Tomassini *et al., PPCF, accepted*
Tomassini *et al., PRAB, submitted*]

The REMPI scheme



Optimization of the injection scheme

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

Very different largest and smallest length scales and we only want to see the slow ones

Reduced models very recommended

Strategy

QFluid

- Fast computational tool for a parameter scan
- Very reduced model: quasistatic approximation, plasma fluid description, 2D cylinidrical simmetry
- Runs on a laptop

ALaDyn

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

[Tomassini *et al.*, PRAB, *submitted*]

Working point

[Tomassini *et al.*, PRAB, *submitted*]

$E_{max}/E_{WB} \sim 1$

$n_0 = 1.1 \times 10^{18}\mathrm{cm}^{-3}$

$L_{density} \simeq L_{laser}$

$L_{charging} \simeq 100\mu\mathrm{m}$

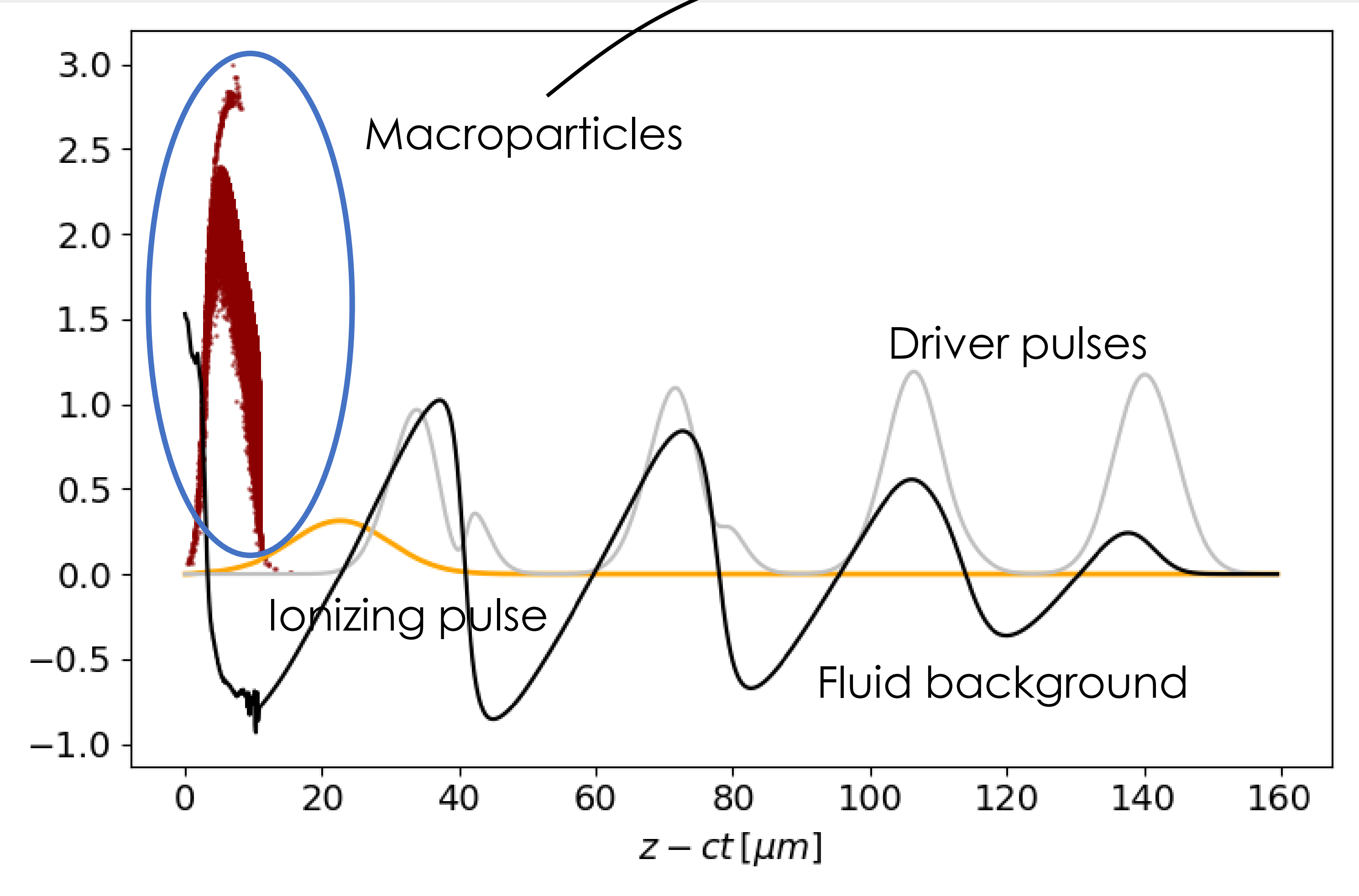
Criticalities

- Fluid model
- Self charge/beam loading
- Quasistatic approximation
- Transverse motion near the axis

Obtained with QFluid → Verified with ALaDyn in **hybrid configuration**

	$\sigma(\mathcal{E})/\mathcal{E}$	ε_n (nm rad)	Twiss γ (m^{-1})	Q (pC)	I (kA)
Requested	<< 5 %	<< 1	< 200	≥ 30	>1
Obtained	1.65 %	0.23	140	32	4

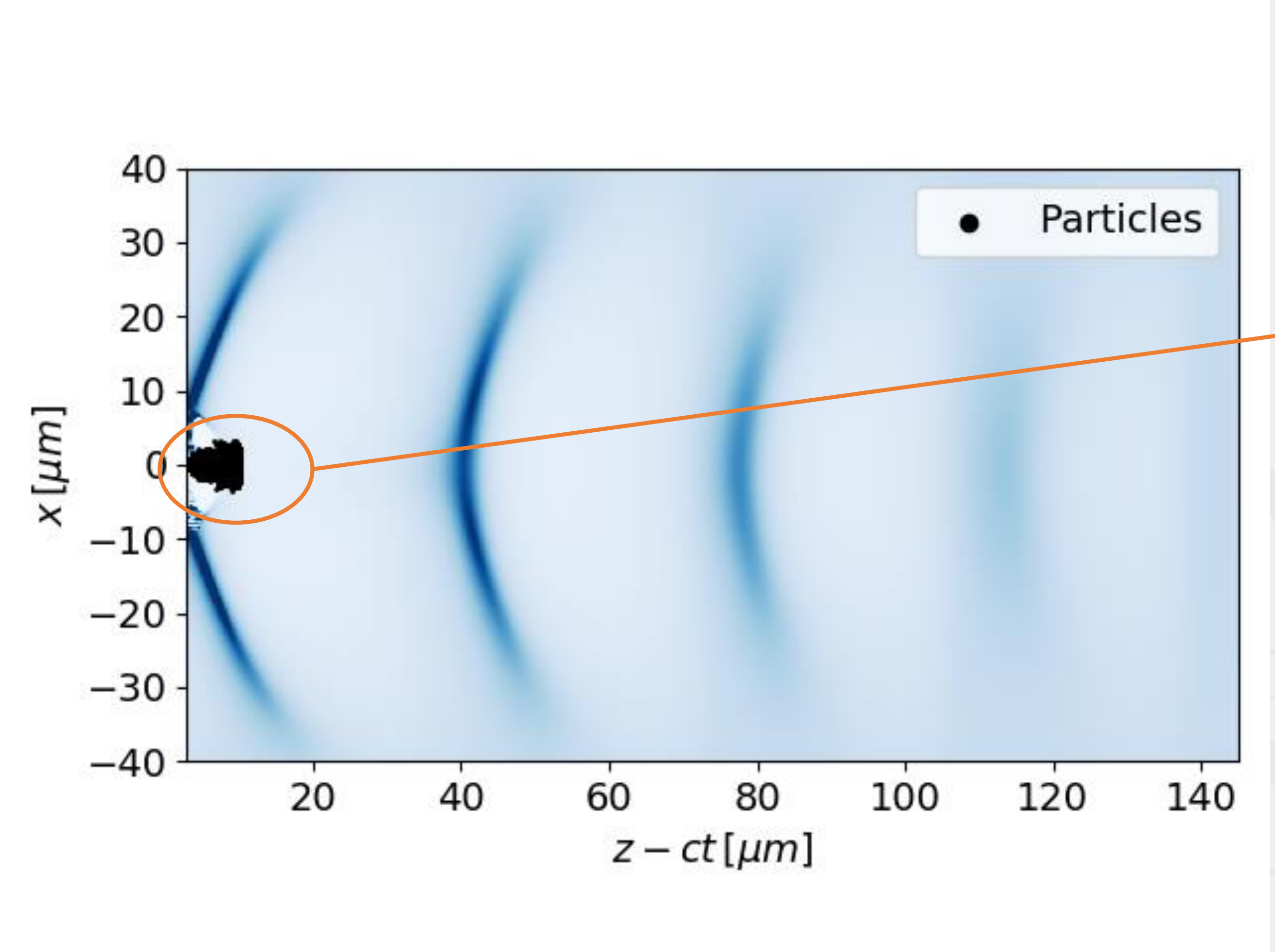
Hybrid simulation



Particles are ionized from the ion background (numerically generated) and injected into the wakefield

Kinetic particles (standard PIC) are moving in a fluid framework

Hybrid simulation/2

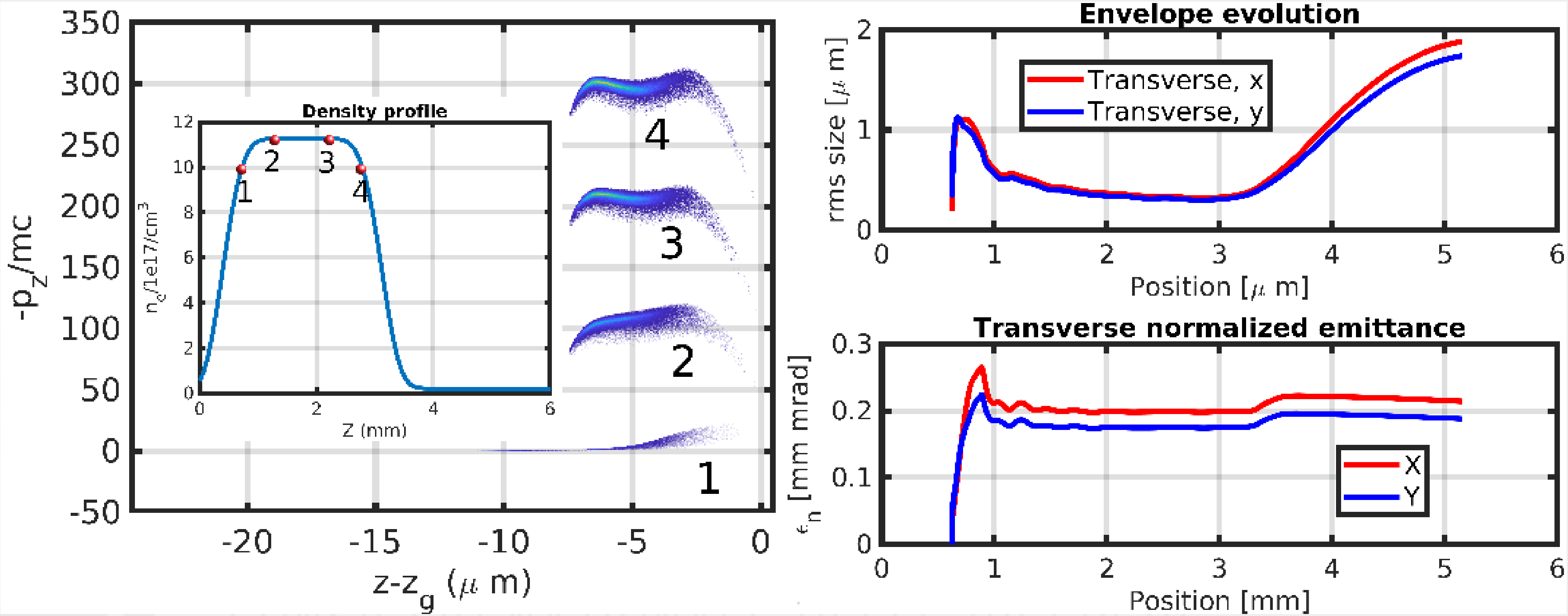


Density map + injected particles

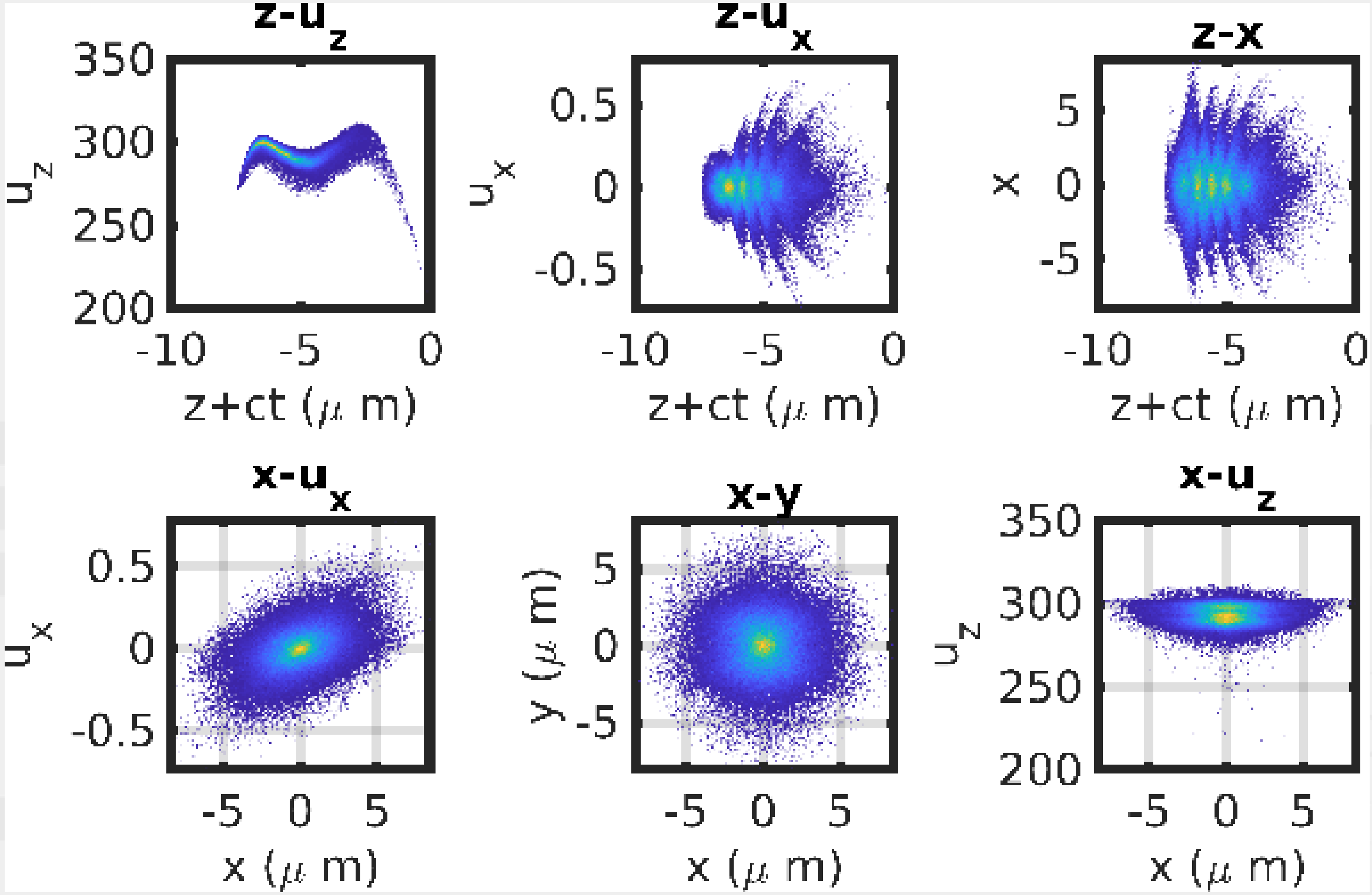
Macroparticles generated via ionization are forming the **accelerating beam**, moving in a fluid density

Simulation time is strongly reduced because particles are only evolved where needed. Of course this could determine some **load unbalance**

Outcomes of the REMPI scheme



Outcomes of the REMPI scheme/2



At the end of the plateau

$$\mathcal{E} = 150\text{MeV}$$

$$\varepsilon_x = 0.21\text{mm} \times \text{mrad}$$

$$\varepsilon_y = 0.23\text{mm} \times \text{mrad}$$

$$\sigma(\mathcal{E})/\mathcal{E} = 1.6\%$$

Conclusions

- **Envelope approximation** allows to model LWFA without any loss of the interesting physics
    - **Explicit** laser solver
    - Approximated **particle pusher**
- **Fluid approximation** greatly boost simulations where fluid theory holds (no kinetic effects)
    - Execution time $\tau \sim 1$ p.p.c.
    - Physics is entirely **retained**
    - **WENO** schemes can offer a flexible, easy and robust option for integration
    - For **strongly nonlinear regimes** a hybrid approach (fluid + few macroparticles) is a promising alternative. **WARNING:** correctness of the results and time gains must be evaluated case by case
- **REMPI** scheme is very demanding in terms of computational time
    - Preliminary parameter scan with **QFLUID**
    - **ALaDyn** in fluid + ionized macroparticles configuration to simulate physics with more accuracy

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