

Modeling Laser Wakefield Acceleration: basic and advanced techniques

Francesco Massimo

Atelier Calcul GdR SCIPAC,

16-18 oct 2024, IJClab

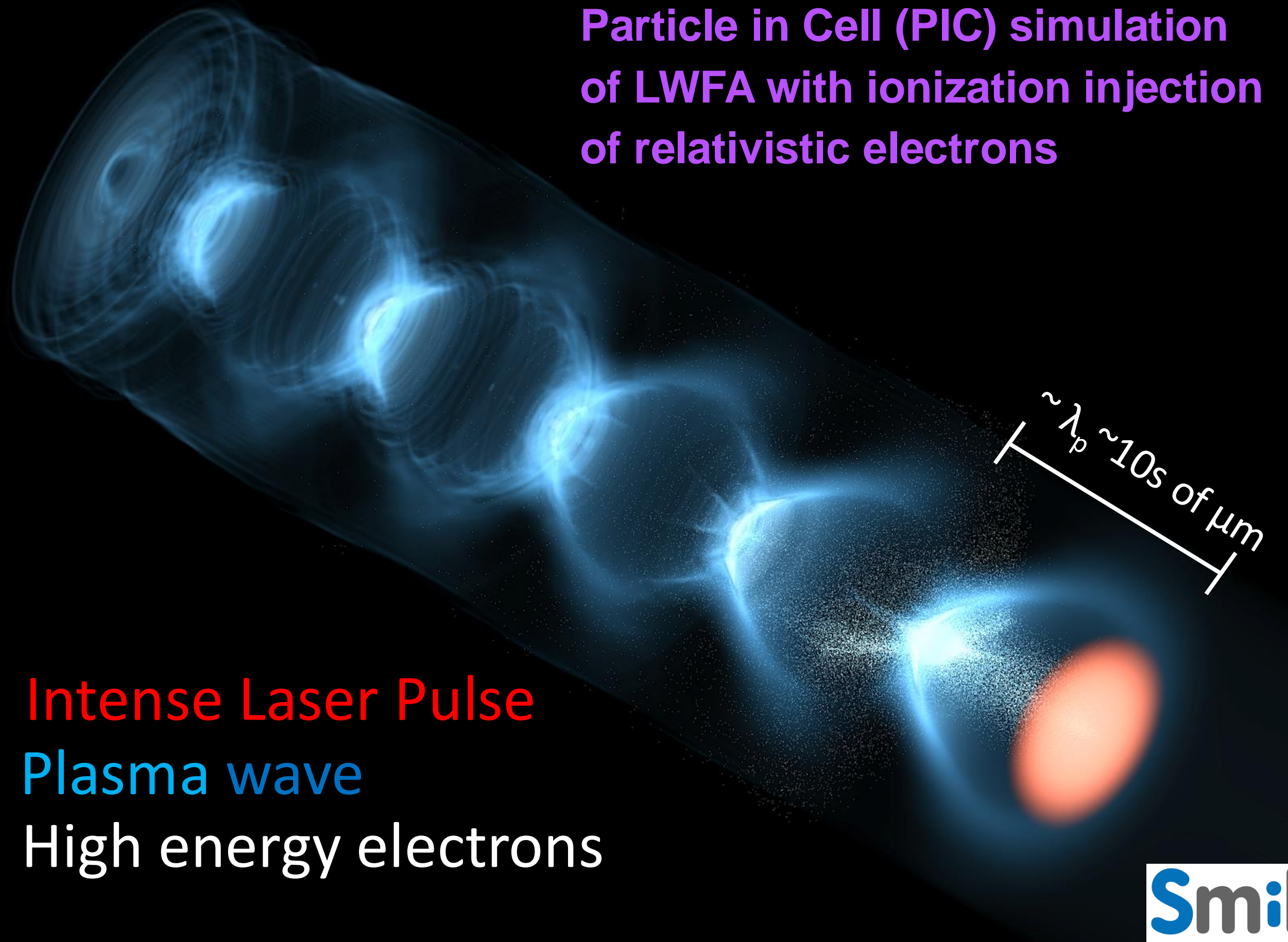
Plan

- Laser Wakefield Acceleration (LWFA): physics scales
- Problem reduction techniques:
 - Cylindrical geometry with azimuthal modes decomposition
 - Laser envelope model
 - Boosted frame
 - Quasi-static approximation
- LWFA modeling challenges

WARNING:
the orders of magnitude
of the speed-ups
are only indicative and case-specific

WARNING: only PIC codes used in the GdR SCIPAC will be mentioned, but many others exist

Particle in Cell (PIC) simulation
of LWFA with ionization injection
of relativistic electrons

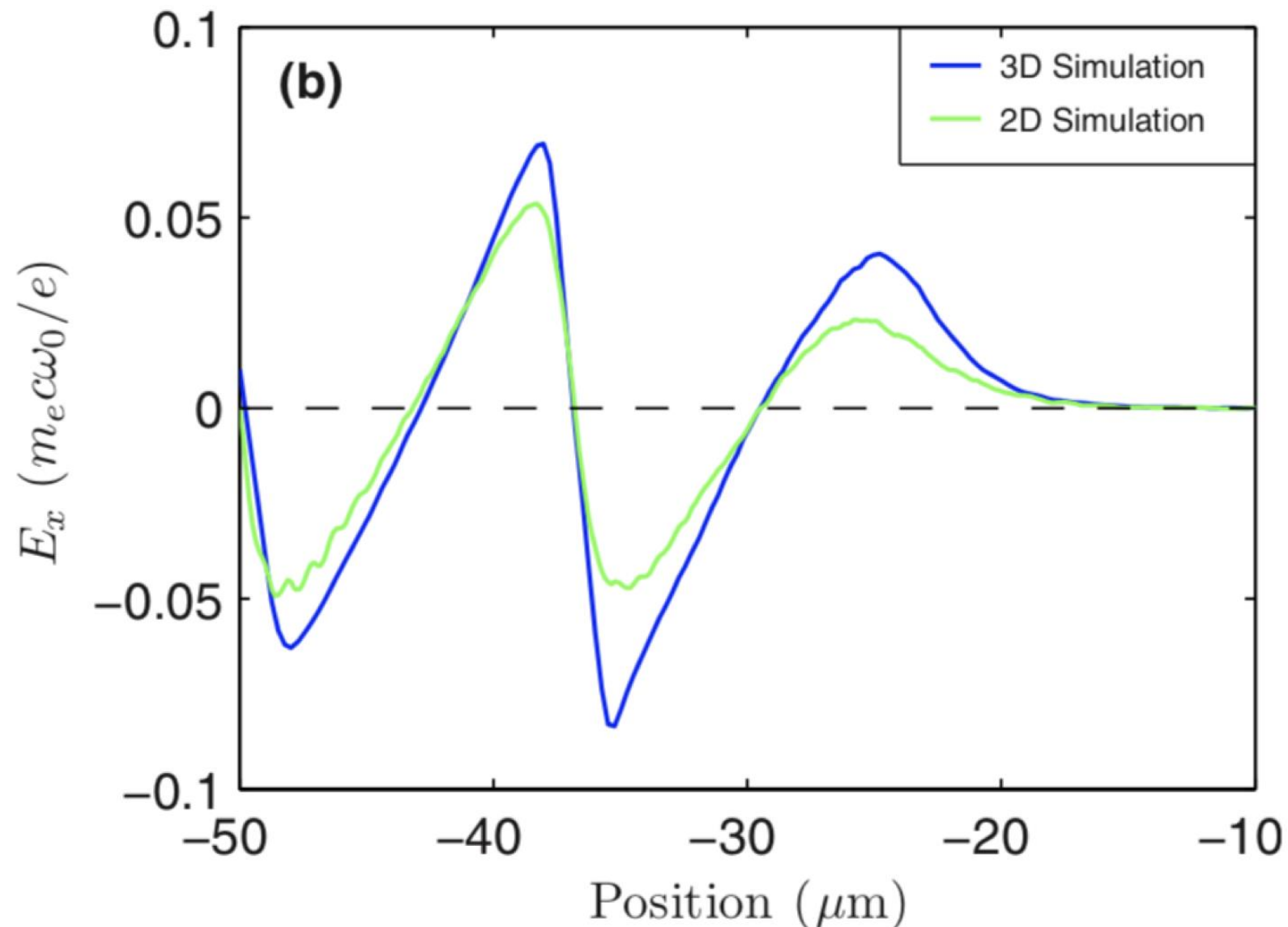


Intense Laser Pulse
Plasma wave
High energy electrons



The LWFA 3D PIC simulation problem is enormous

2D cartesian simulations:
Not accurate enough



X. Davoine et al., Phys. Plasmas 15, 113102 (2008)

Example of 3D simulation scale
with “classic” electromagnetic PIC loop
and “classic” numerical schemes

- Laser wavelength $\lambda_0 = 0.8 \mu\text{m} \rightarrow 0.016 \mu\text{m}$, $\Delta x = 0.016 \mu\text{m}$, $c\Delta t = 0.99\Delta x$
- Laser duration: 30 fs \rightarrow Window size $L_x = 40 \mu\text{m} = 2500 * \Delta x$
- $w_0 = 12 \mu\text{m} \rightarrow \Delta y = \Delta z = 0.5 \mu\text{m}$, Window size $L_y = L_z = 125 \mu\text{m} = 192 * \Delta y$
- Acceleration length = 1 mm $\sim 60000 c * \Delta t$
- 8 macro-particles per cell $\rightarrow \sim 2500 * 250 * 250 * 8 =$

10^9 macro-particles, pushed for 60k timesteps!

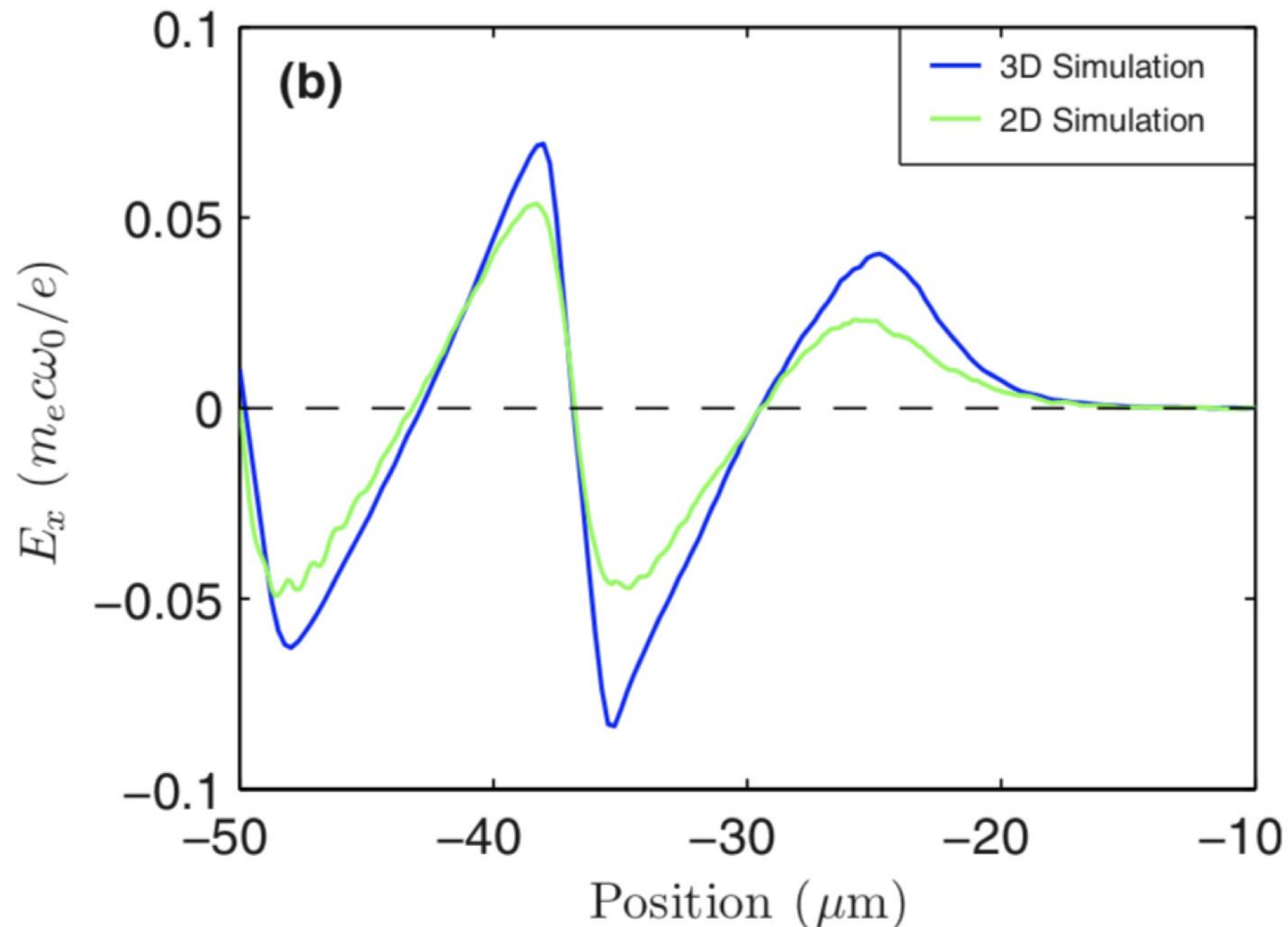
Exemple of full 3D simulation:

1 Mh-cpu/cmon Jean-Zay Cascadelake 2019

(ask Arnaud Beck!)

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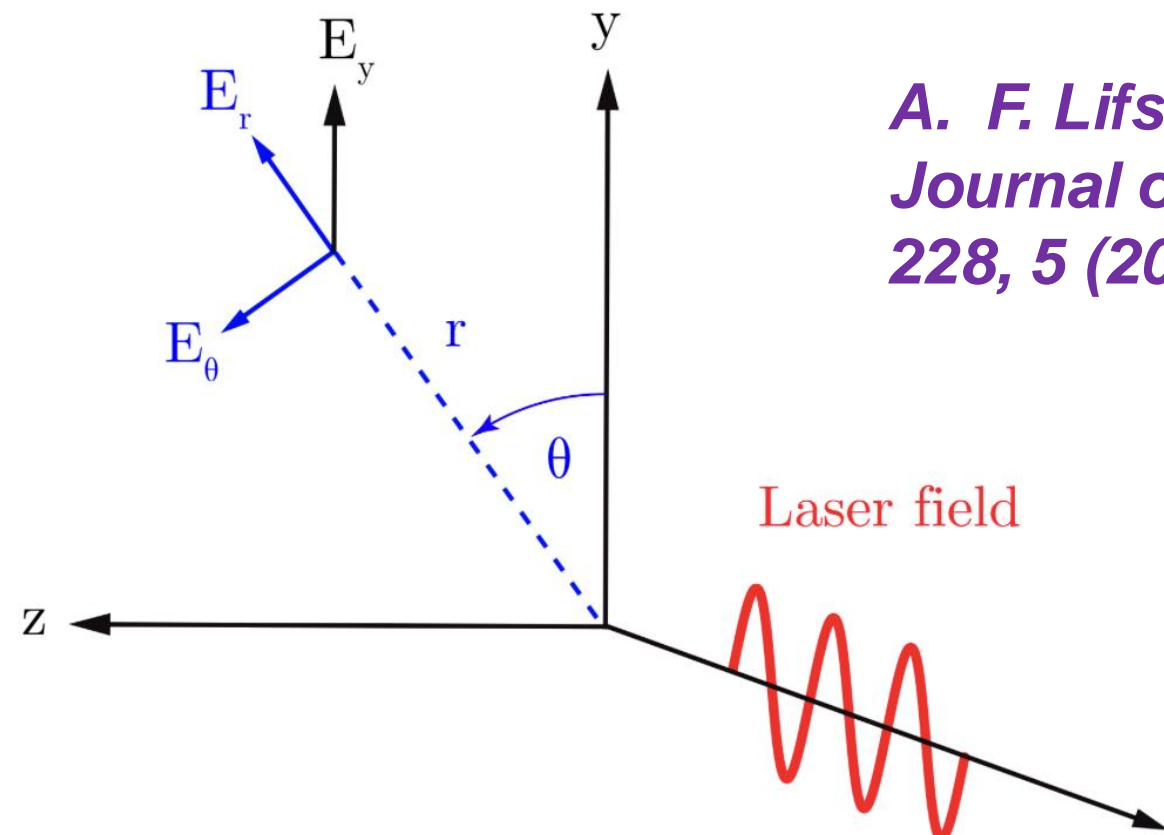
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**Smallest scale
to sample
[space and time]**

**Largest scale to simulate
[space and time]
(Note: current LWFA studies
require several mm, up to
10s of cm, or even m)**

Cylindrical geometry with azimuthal modes decomposition

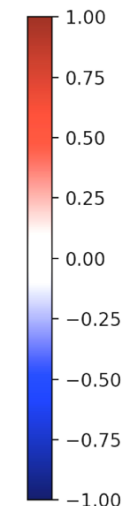
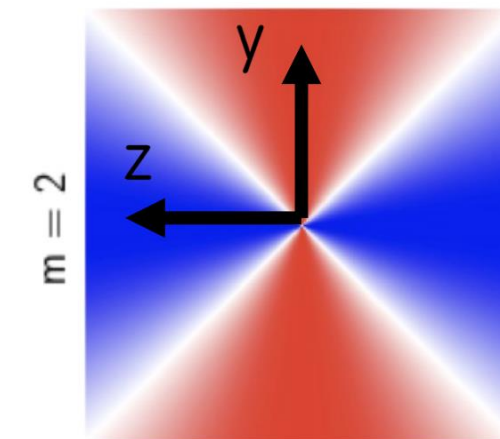
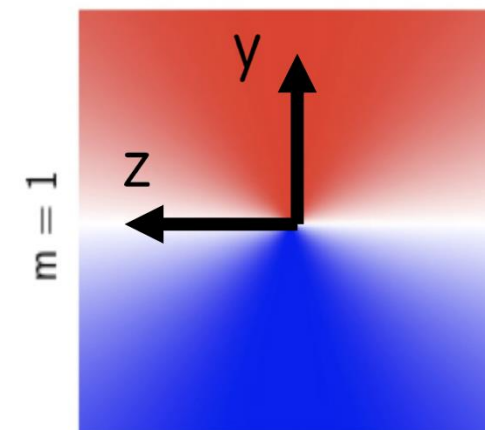
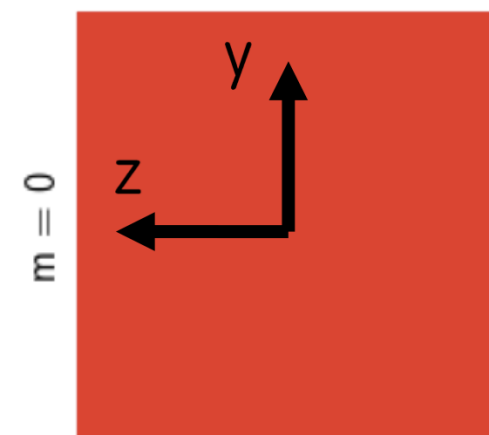


A. F. Lifschitz et al.,
Journal of Computational Physics
 228, 5 (2009)

2D Cylindrical grids instead of 3D cartesian grids

$$F(x, r, \theta) = \text{Re} \left[\sum_{m=0}^{+\infty} \tilde{F}^m(x, r) \exp(-im\theta) \right]$$

Any scalar field or vector field component in cylindrical coordinates

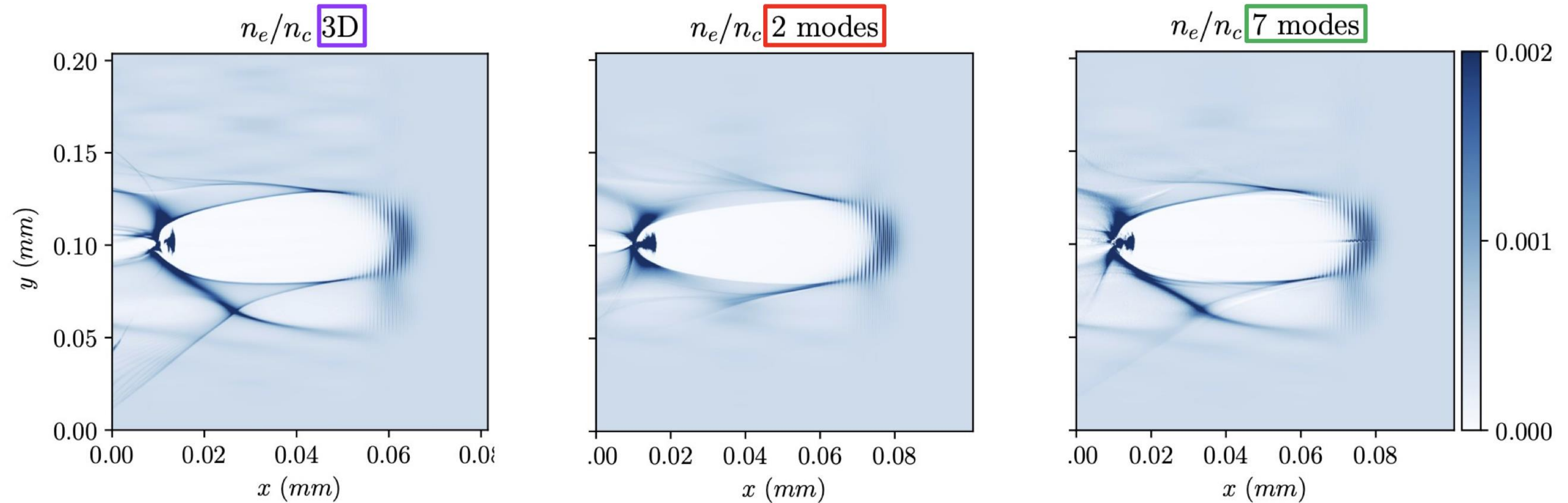


Re $[\exp(-im\theta)]$

Examples of PIC codes in SCIPAC:

CALDER-CIRC, Smilei, FB-PIC, WarpX, Wake-T ($m=0$)

Cylindrical geometry with azimuthal modes decomposition

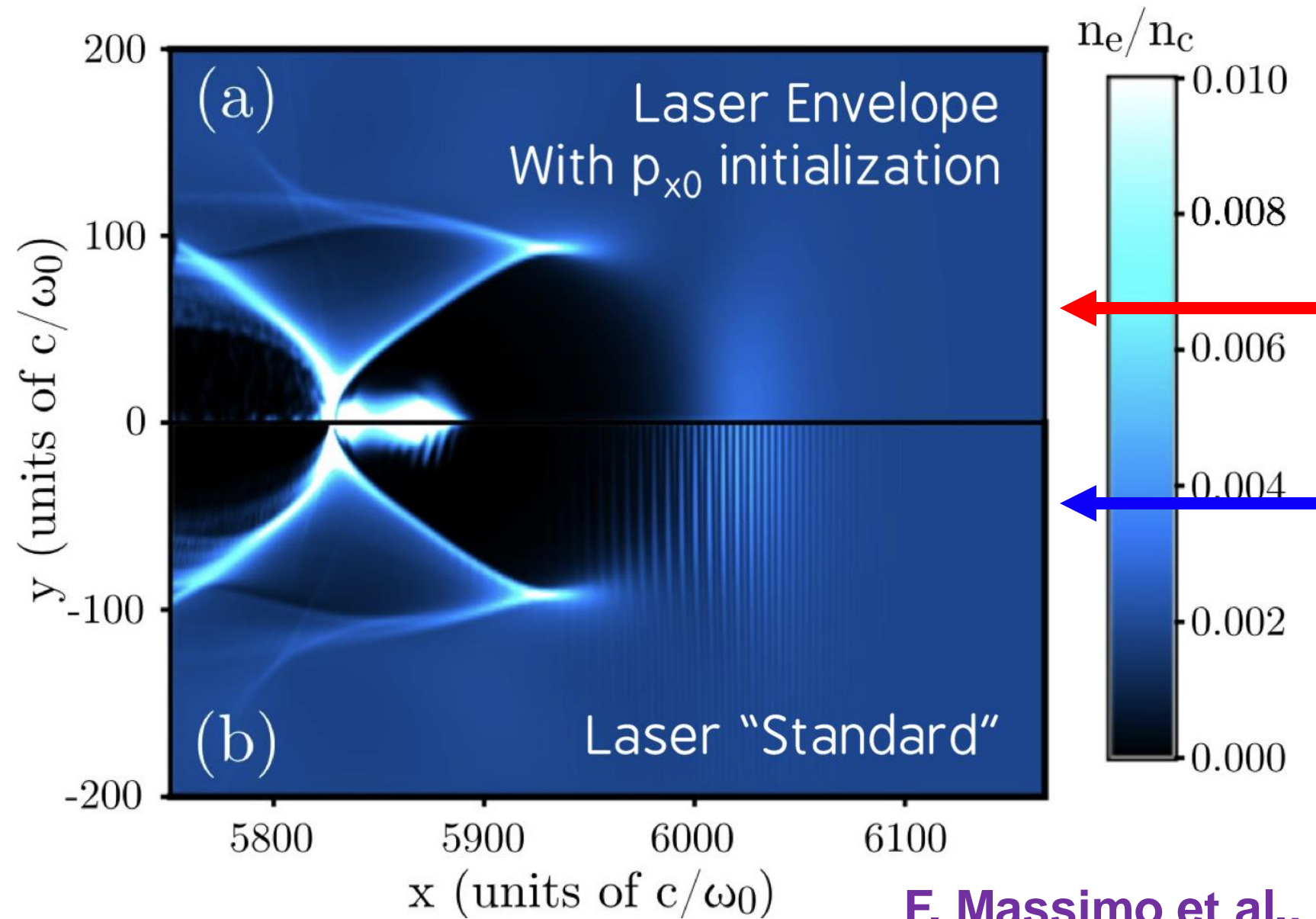


I. Zemzemi, PhD thesis, <https://theses.fr/2020IPPAX111>

Speed-up $\sim (ppc_y * ppc_z * N_{\text{grid},\perp}) / (N_{\text{modes}} * ppc_r * ppc_\theta) \sim 10-100$ (case-specific)

(N_{modes} typically < 5 , and $ppc_\theta \sim 4 * N_{\text{modes}}$ for $N_{\text{modes}} > 1$)

Laser Envelope modeling



Envelope simulation Δx : resolves $c \cdot T_{\text{laser}}$
Envelope simulation Δt : resolves T_{laser}

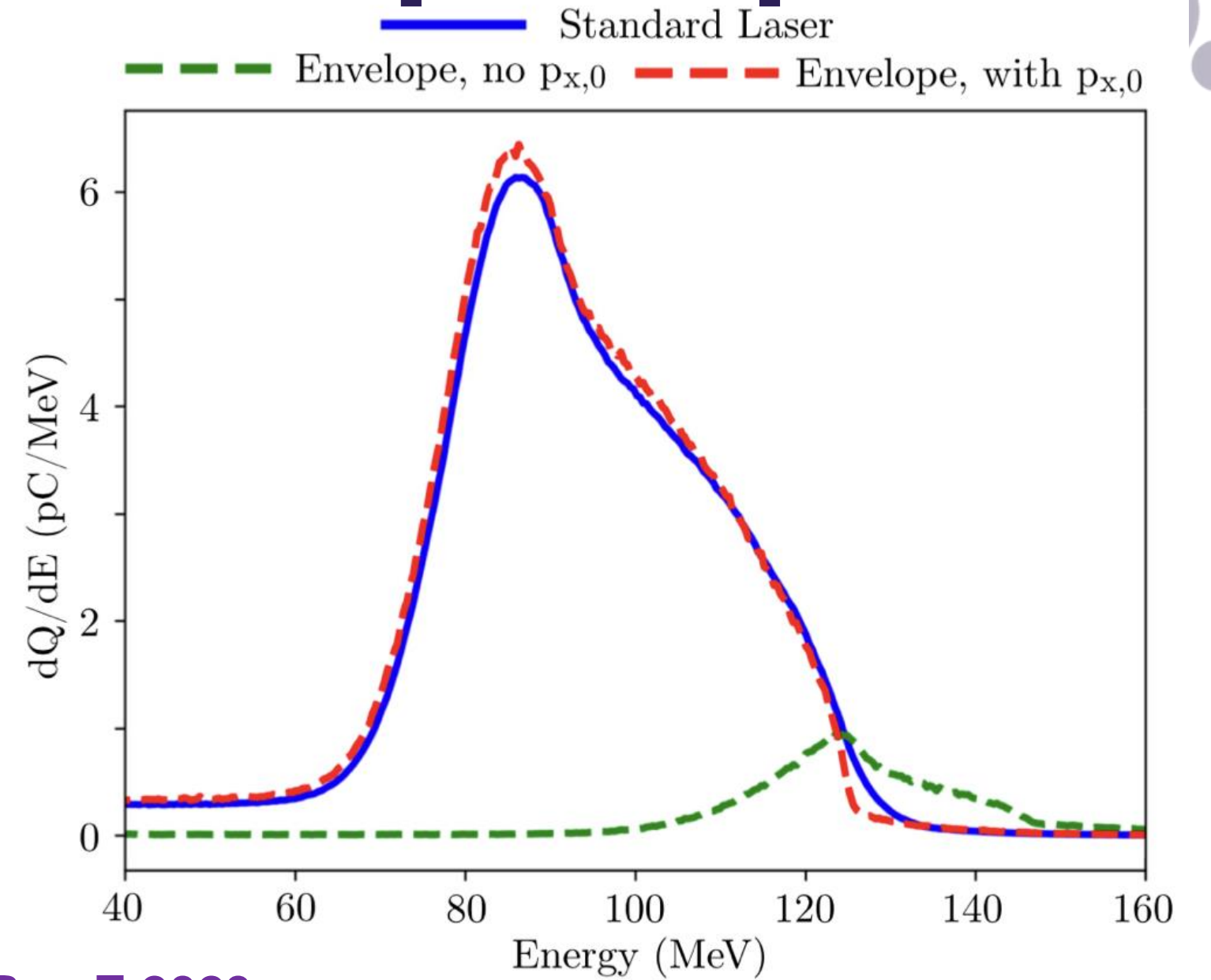
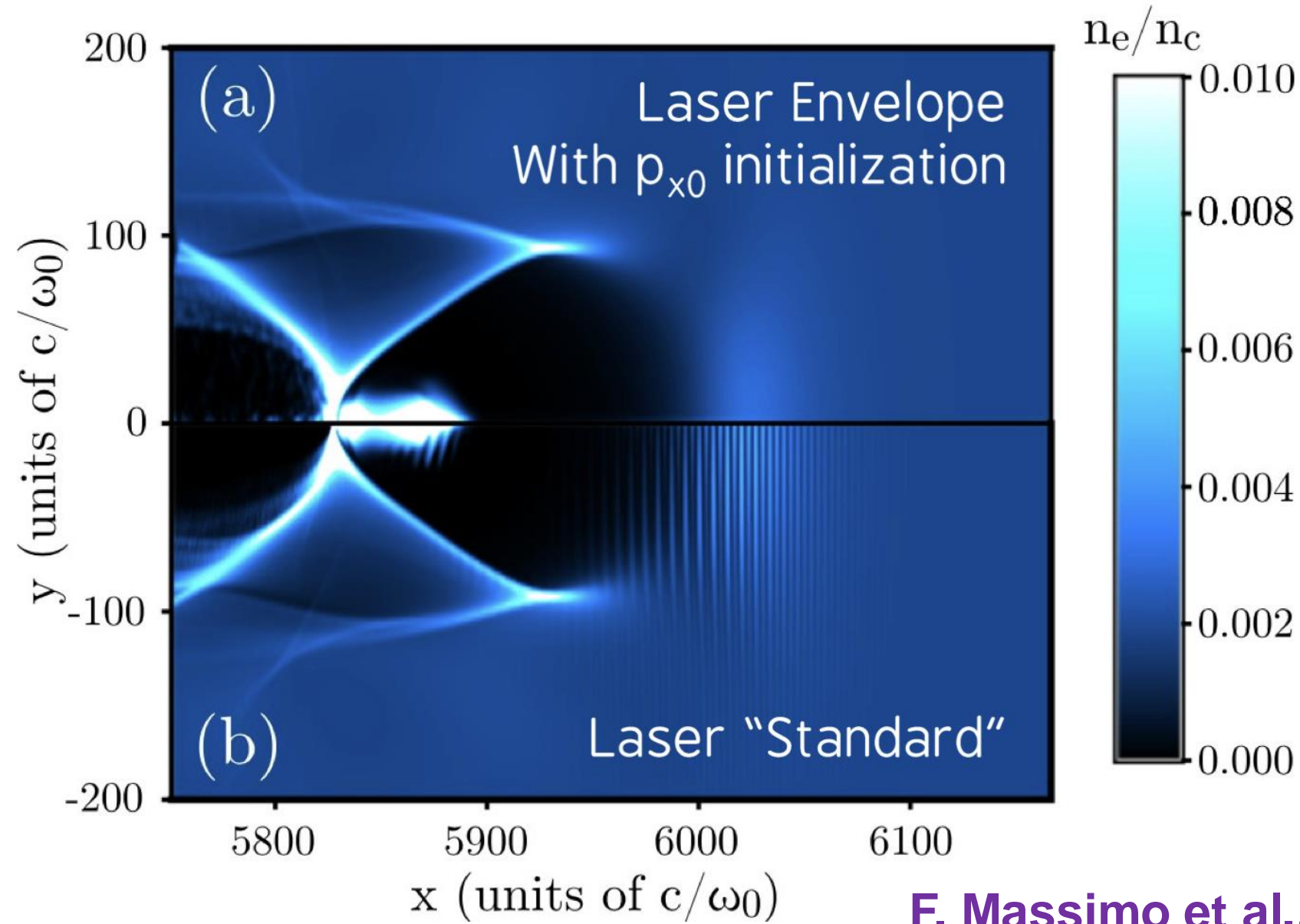
"Standard" simulation Δx : resolves λ_0
"Standard" simulation Δt : resolves λ_0/c

F. Massimo et al., Phys. Rev E 2020

Examples of PIC codes in SCIPAC:

Smilei, HiPACE++ (quasi-static), Wake-T (quasi-static, $m=0$)

Laser Envelope modeling: results and speed-up

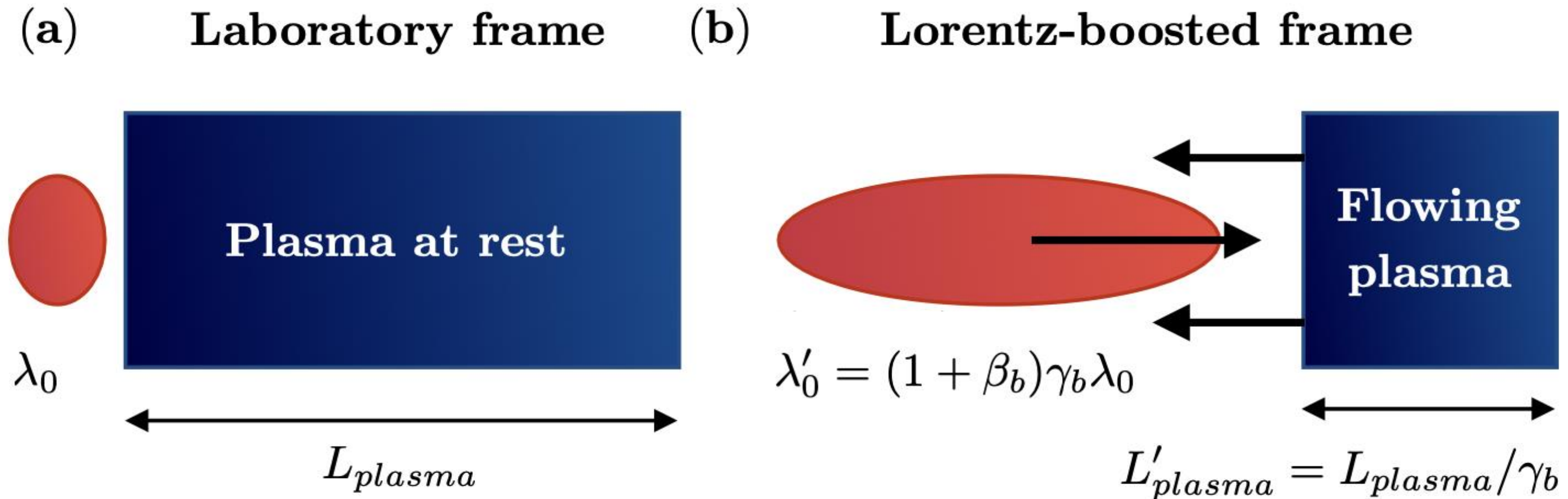


F. Massimo et al., Phys. Rev E 2020

Speed-up $\sim (cT_{\text{laser}})^2/(\lambda_0)^2 \sim n_{\text{critical}}/n_{\text{plasma}} \sim 10-100$ (case-specific)

[in cylindrical symmetry you can even use 1 macro-particle per cell for first scans
see also **P. Drobniak et al., Phys. Rev. Accel. Beams 26, 091302 (2023)**]

Lorentz boosted frame: reducing the LWFA problem size



P. Lee, PhD thesis (2017)

<https://theses.hal.science/tel-01581770>

Examples of PIC codes in SCIPAC: FB-PIC, WarpX

Lorentz boosted frame: speed-up

Ideal speed-up given by:

- shorter interaction time
- Coarser longitudinal and temporal resolution

$$\rightarrow \gamma_b^2 (1 + \beta_b)^2$$

when $L_{\text{prop}}/L_{\text{window}} \gg 1$

And $\beta_{\text{window}} \rightarrow 1$

Factors that can reduce the **real speed-up**:

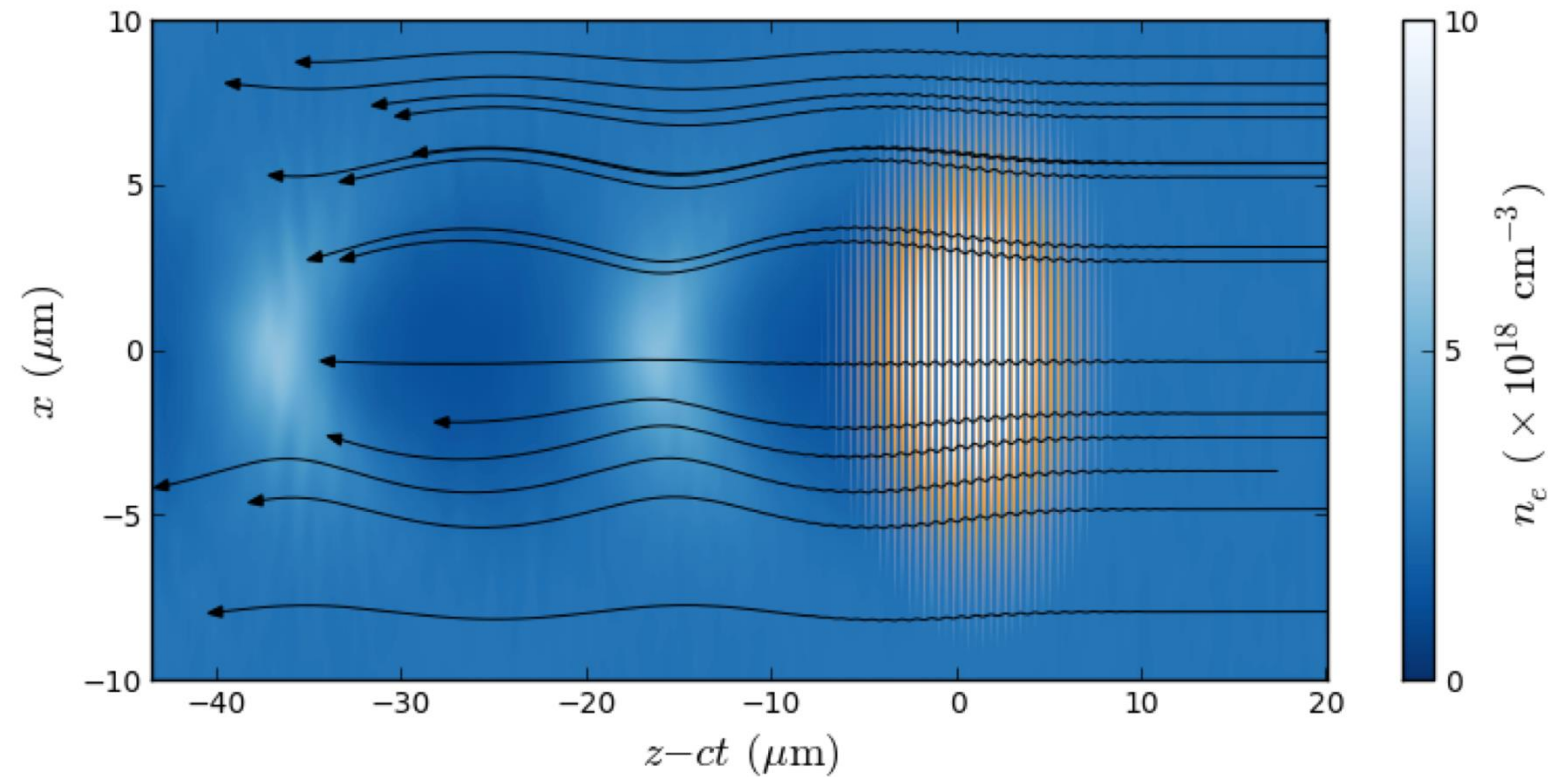
- Stability of your solvers with different resolution
- Numerical Cherenkov instability
- Too many diagnostics
- Plasma becoming overdense in the boosted frame
- Resolution not suited for sampling plasma wave
- Slower moving window (\rightarrow lower β_{window})
- ...

More realistic speed-up analysis in

https://fbpic.github.io/advanced/boosted_frame.html

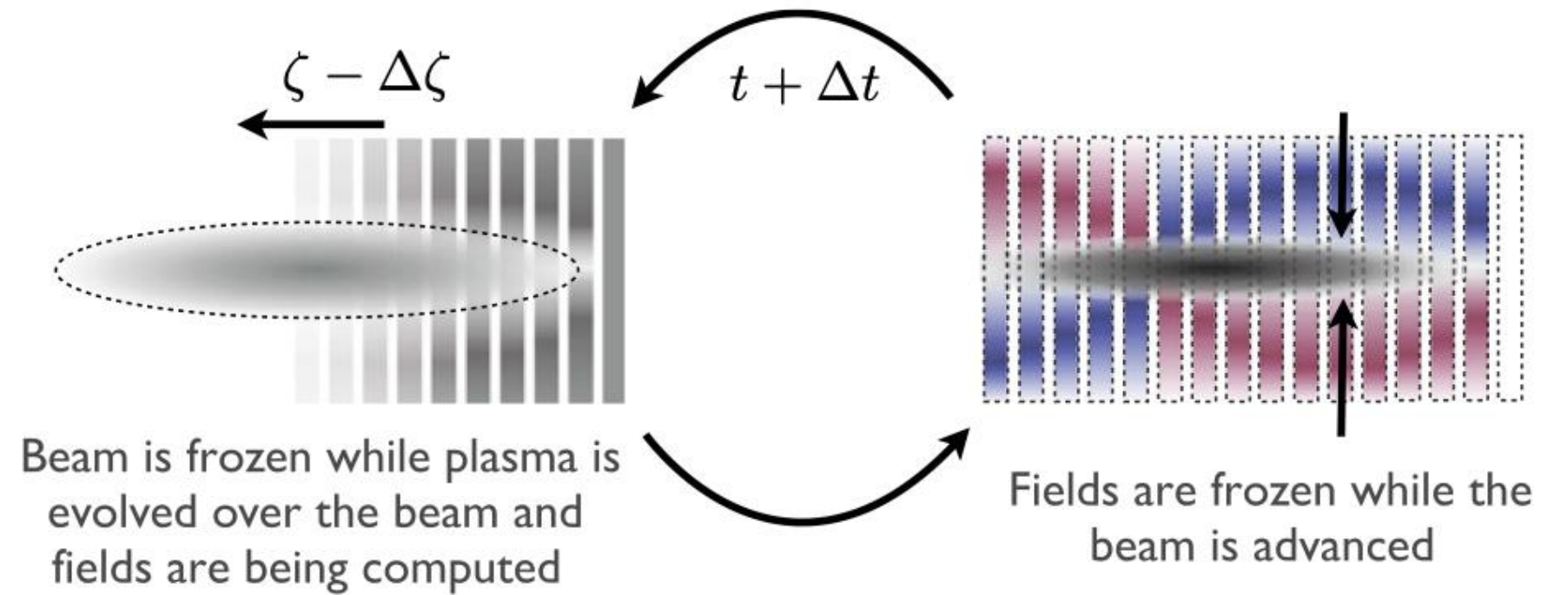
Speed-up ~ 10-100 (case-specific)

Quasi-static approximation



R. Lehe, PhD thesis
<https://pastel.hal.science/tel-01088398>

Quasi-static PIC loop



T. Mehrling *et al*, *Plasma Phys. Control. Fusion* (2014)

Speed-up $\sim (n_{\text{critical}}/n_{\text{plasma}})^{3/2} \sim 1000$ (case-specific)

Examples of PIC codes in SCIPAC:

HiPACE++ (envelope), Wake-T (envelope, actually with a reduced wakefield LWFA model)

LWFA Modeling challenges (list far from complete...)

Note: this classification is arbitrary, these categories intersect each other

Capturing the underlying physics:

- Coupling different problem reduction techniques
- Multi-code (multi-physics) couplings
- Using experimentally characterized laser fields as inputs
- Benchmarking problem reduction models at extreme conditions
- Coupling with machine learning

Numerical effects:

- Numerical Cherenkov instability
- Numerical Dispersion
- Boundary conditions to remove border wave reflections
- Axis management in cylindrical geometry

Parallelization and Software Engineering:

- Load imbalance at different levels
- Managing different CPU and GPU architectures
- Development, maintenance, scalar debt of software with many features

Conclusions

- LWFA PIC modeling requires 3D (or 3D-like) accuracy, but this requires lots of computational resources
- Typical techniques used to reduce the problem size:
 - Cylindrical geometry with azimuthal modes decomposition
 - Laser envelope modeling
 - Lorentz boosted frame
 - Quasi-static approximation
- Sometimes these techniques can also be coupled (e.g. cylindrical geometry+envelope modeling)
- Many LWFA modeling challenges exist, related to the physical models, numerical schemes, parallelization and software engineering, often intersecting each other